High Production Volume (HPV) Chemical Challenge Program:
Final Revised Test Plan and Assessment with Robust Study Summaries
for
Linear and Branched Alkylbenzene Sulfonic Acids and Derivatives
Part II: Robust Study Summaries for LAS/ABS Category

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8 Robust Study Summaries for LAS/ABS Category

Every available study and endpoint estimate included in Section 5 tables and text is summarized in the Appendix. Each robust study summary includes a reference number that matches the reference number in Section 7.2 as well as a reliability score based on the Klimisch criteria described in Section 3.0. The studies are presented by CAS Number within each endpoint and the CAS Number order is consistent for each of the endpoints.

8.1 Physical-Chemical Endpoints

8.1.1 Melting Point

CAS No. 27176-87-0

(a)

Value:	-10 degrees C
Method:	Not specified
GLP:	Yes **[ ]** No **[]** ? **[X]**
Test Substance:	Benzenesulfonic acid, dodecyl- (CAS RN **27176-87-0**)
Remarks:	IUCLID cites source as Hoechst Iberica s.a. Barcelona
Reference:	**74.** European Commission IUCLID Data Set; Benzenesulfonic acid, dodecyl- CAS RN **27176-87-0.** 1995
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.1.2 Boiling Point

CAS No. 26264-05-1

(a)

Value:	>149 degrees C
Method:	Not specified
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1), purity 90%
Remarks:	At 1.0E5 Pa
Reference:	**22.** Rhodia MSDS RHODOCAL®330. 1998
Reliability:	4 Not assignable. Secondary literature.

CAS No. 68953-96-8

(a)

Value:	117 degrees C
Method:	Not specified
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., calcium salts; purity 69.5-71.5%
Remarks:	Tested as a formulation containing 77% HPV substance plus organic solvent.

Reference: **3,4.** Harcros MSDS and product specification Casul 55HF and Casul 70HF. 2000
Reliability: 4 Not assignable. Secondary literature.

CAS No. 27176-87-0
(a)
Value: 205 degrees C at 1013 hPa
Method: Not specified
GLP: Yes **[ ]** No **[]** ? **[X]**
Test Substance: Benzenesulfonic acid, dodecyl- (CAS RN **27176-87-0**)
Remarks: **74.** IUCLID cites source as Hoechst Iberica s.a. Barcelona
Reference: European Commission IUCLID Data Set; Benzenesulfonic acid, dodecyl- CAS RN **27176-87-0.** 1995
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.1.3 Vapor Pressure

CAS No. 26264-05-1
(a)
Value: <3.1E3 Pa (=3,100 Pa)
Method: Not specified
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1), purity 90%
Remarks: Temperature = 25 degrees C.
Reference: **22.** Rhodia MSDS RHODOCAL®330. 1998
Reliability: 4 Not assignable. Secondary literature.

CAS No. 27323-41-7
(a)
Value: 1.06E-024 mm Hg (= $8x10^{27}$ Pa)
Method: Estimated by Calculation
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: CAS No. **27323-41-7;** benzenesulfonic acid, dodecyl-, compd. with 2,2',2"-nitrilotris[ethanol]
Remarks: Molecular formula C24H45NO6S; Molecular weight = 476. Temperature = 25 degrees C. Estimate made using SRC software. Equivalent to $8x10^{27}$ Pa (conversion of 1 mm Hg = 133 Pa)
Reference: **71.** Syracuse Research Corporation (SRC) PhysProp Database. Neely, WB and Blau, GE, 1985.
Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68953-96-8

(a)

Value:	733 Pa
Method:	Not specified
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., calcium salts; purity 69.5-71.5%
Remarks:	Temperature = 20 degrees C.
Reference:	**3,4.** Harcros MSDS and product specification Casul 55HF and Casul 70HF. 2000
Reliability:	4 Not assignable. Secondary literature.

CAS No. 68411-30-3

(a)

Value:	$3x10^{-13}$ Pa
Method:	Calculation
Test Substance:	Benzenesulfonic acid, C10-13 alkyl derives., sodium salt
Remarks:	Estimates calculated by Lyman, W.J, 1985. Environmental Exposure from Chemicals. Vol 1, p.31. CRC Press. Boca Raton.
Reference:	**43.** European Commission. Cited in IUCLID Datasheet for CAS # 68411-30-3. Year 2000 CD ROM Edition.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.1.4 Partition Coefficient: $\log_{10}P_{ow}$ ($\log_{10}K_{ow}$)

CAS No. 26264-05-1

(a)

Log Pow:	6.18
Method:	Estimated by Calculation
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1),
Remarks:	Molecular formula C21H38NO3S; Molecular weight = 385.
Reference:	**83.** USEPA. KOWWIN version 1.67. EPI Suite version 3.20. February 2007
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 27323-41-7

(a)

Log Pow:	1.85
Method:	Estimated by Calculation
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	benzenesulfonic acid, dodecyl-, compd. with

2,2',2"-nitrilotris[ethanol]

Remarks: Molecular formula C24H45NO6S; Molecular weight = 476. Estimate made using SRC software.

Reference: **84.** Syracuse Research Corporation (SRC) PhysProp Database. Meylan, WM and Howard, PH, 1995.

Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 27323-41-7

(a)

Log Pow: 1.85

Method: Estimated by Calculation

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test Substance: benzenesulfonic acid, dodecyl-, compd. with 2,2',2"-nitrilotris[ethanol]

Remarks: Molecular formula; C24H45NO6S; Molecular weight = 476.

Reference: **83.** USEPA. KOWWIN version 1.67. EPI Suite version 3.20. February 2007

Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 26264-06-2

(a)

Log Pow: 6.78

Method: Estimated by Calculation

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test Substance: Benzenesulfonic acid, dodecyl-, calcium salts with 2,2',2"-nitrilotris[ethanol]

Remarks: Molecular formula; C18H30O3SCa; Molecular weight = 367.

Reference: **83.** USEPA. KOWWIN version 1.67. EPI Suite version 3.20. February 2007

Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68953-96-8

(a)

Log Pow: 5.54

Method: Estimated by Calculation

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test Substance: Benzenesulfonic acid, mono-C11-13 –branched alkyl derives., calcium salts

Remarks: Molecular formula; C18H30OS; Molecular weight = 295.

Reference: **83.** USEPA. KOWWIN version 1.67. EPI Suite version 3.20. February 2007

Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68411-30-3

(a)

Log Pow:	3.32
Method:	Estimated by Calculation
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	$C_{11.6}$ LAS
Remarks:	Calculated for $C_{11.6}$ LAS using the QSAR method of Leo and Hansch (1979) as modified by Roberts (1991) for surfactant structures. This takes into account the various phenyl positions along the linear alkyl chain. See the Roberts (1991) summary at 2.5(g) for a full description of the method modifications.
Reference:	**42.** (1) HERA. 2004. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. **68411-30-3**, Version 2.0 June 2004. http://www.heraproject.com/riskassessment.cfm. 2) Leo, A.J. and Hansch, C. 1979. Substituent Constants for Correlation Analysis in Chemistry and Biology. J. Wiley & Sons, NY 3) Roberts, D.W. 1991. QSAR issues in aquatic toxicity of surfactants. Sci. Total Environ. 109/110:557-568.
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

(b)

Log Pow:	2.02
Method:	Estimated by Calculation
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	Benzenesulfonic acid, C10-13 alkyl derives., sodium salt
Remarks:	Molecular formula; C16H25O3SNa; Molecular weight = 320.
Reference:	**83.** USEPA. KOWWIN version 1.67. EPI Suite version 3.20. February 2007
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 27176-87-0

(a)

Log Pow:	1.96
Method:	other (calculated): Leo and Hansch
GLP:	Yes **[ ]** No **[]** ? **[X]**
Test Substance:	Benzenesulfonic acid, dodecyl- (CAS RN **27176-87-0**)
Remarks:	original data from Leo, A, Hansch, C and Elkins D. 1971. Chem. Rev. 71:525-616.
Reference:	**76.** Hand, V.C. and Williams, G.K. 1987. Structure activity relationships for sorption of linear alkylbenzenesulfonates. Environ. Sci. Technol. 21:370-373.
Reliability:	2 Valid with restrictions. Data from standard reference source.

CAS No. 27176-87-0

(a)

Log Pow:	4.78
Method:	Estimated by Calculation
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	Benzenesulfonic acid, dodecyl-
Remarks:	Molecular formula; C18H30O3S; Molecular weight = 327.
Reference:	**83.** USEPA. KOWWIN version 1.67. EPI Suite version 3.20. February 2007
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

8.1.5 Water Solubility

CAS No. 26264-05-1

(a)

Value:	dispersable
Method:	Not specified
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1), purity 90%
Remarks:	none
Reference:	**22.** Rhodia MSDS RHODOCAL®330. 1998
Reliability:	4 Not assignable. Secondary literature.

CAS No. 27323-41-7

(a)

Value:	27.1 mg/L
Method:	Estimated by Calculation
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	CAS No. **27323-41-7;** benzenesulfonic acid, dodecyl-, compd. with 2,2',2"-nitrilotris[ethanol]
Remarks:	Molecular formula C24H45NO6S; Molecular weight = 476. Temperature = 25 degrees C. Estimate made using SRC software.
Reference:	**71.** Syracuse Research Corporation (SRC) PhysProp Database. Meylan, WM et. al.,1996.
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 26264-06-2

(a)

Value:	dispersable
Method:	Not specified
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	Benzenesulfonic acid, dodecyl-, calcium salts
Remarks:	none

Reference: **21.** Rhodia MSDS RHODOCAL®CA/70. 1998.
Reliability: 4 Not assignable. Secondary literature.

CAS No. 68953-96-8
(a)
Value: dispersible.
Method: Not specified
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., calcium salts; purity 69.5-71.5%
Remarks: none
Reference: **3,4.** Harcros MSDS and product specification Casul 55HF and Casul 70HF. 2000
Reliability: 4 Not assignable. Secondary literature.

CAS No. 68411-30-3
(a)
Value: ca. 250 g/L
Method: Not specified
Temperature: 20°C
Description: Miscible in water
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: Marlon A 390 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks: Miscible with water at 20°C. Depending on the concentration, clear solutions (up to ~25% w/w) or inhomogeneous, viscous pastes were obtained. Sources cited are two reports by Huels AG dated 1988 and 1993.
Reference: **43.** European Commission. IUCLID Data Sheet for CAS # **68411-30-3.** 2000 CD ROM version.
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

CAS No. 27176-87-0
(a)
Value: 300,000 mg/L at 20 degrees C (= 300g/L)
Method: Not specified
GLP: Yes **[ ]** No **[]** ? **[X]**
Test Substance: Benzenesulfonic acid, dodecyl- (CAS RN **27176-87-0**)
Remarks: IUCLID cites source as Shell Chemical report indicating that substance is miscible in water up to 40%.
Reference: **75.** European Commission IUCLID Data Set; Benzenesulfonic acid, dodecyl- CAS RN **27176-87-0.** 1995

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.2 Environmental Fate Endpoints

8.2.1 Photodegradation

CAS No. 68411-30-3

(a)

Type: air [ ]; water [X]; soil [ ]

Light source: sunlight [ ]; xenon lamp [ ]; other [X] mercury vapour lamp

Light spectrum: 200-350 nm

Concentration: initial LAS concentration 60 to 182 mg/L

Temperature: 28 degrees centigrade

Direct photolysis degradation: >95% (weight/weight) in 20 minutes (exposure time)

Indirect photolysis degradation: rapid photodegradation

Method: A series of photodegradation studies were conducted. Aqueous solutions of LAS (pH 6.75) were passed through an irradiated tubular flow reactor. Reaction rates were obtained for both non-sensitized conditions and when ferric perchlorate (0.04 to 3.15 x 10^{-4} g-mole/L) was used as a sensitizer. A Hanovia 1200-watt mercury-vapour lamp was the source of radiation. The LAS concentration was determined by the methylene blue method. Appropriate controls were used.

GLP: Yes [ ]; No [X]

Remarks: Complete conversion of LAS to intermediates at an average residence time as low as one minute. The maximum conversion to CO_2 was obtained at a residence time of 20 minutes and corresponds to 7 moles CO_2 per mole of LAS. Reaction rate increased by two orders of magnitude in presence of ferric perchlorate. Half order kinetics with respect to light intensity and LAS concentration explained the data for nonsensitized conditions. The sensitized reaction was believed to occur by abstraction of hydrogen atoms from LAS by hydroxyl radicals that are presumably produced by an electron-transfer reaction involving light-activated ferric ions. The mechanism is complex; over-all kinetics indicated a first order effect of Fe^{+3} , 1.2 order in light intensity and maxima in the rate for intermediate LAS and O_2 concentrations.

Reference: **80.** Matsuura, T and Smith, JM. 1970. Kinetics of photodecomposition of dodecyl benzene sulfonate. Ing. Eng. Chem. Fund. 9:252-260.

Reliability: 2 Valid with restrictions

8.2.2 Stability in Water (Hydrolysis)

CAS No. 68411-30-3

(a)

Type:	Abiotic (hydrolysis) [X]; biotic (sediment) [ ]
Results:	Stable in water
GLP:	Yes [ ]; No [X]
Test substance:	$C_{10\text{-}13}$ alkylbenzene sulfonic acid, sodium salt (CAS#68411-30-3)
Remarks:	LAS can be decomposed at extreme conditions such as elevated temperatures in the presence of inorganic acids such as phosphoric, sulphuric and hydrochloric (e.g., 60-70% sulphuric acid at 140-190 degrees C or with concentrated HCl in a sealed container at 150-200 degrees C). Information as cited in IUCLID Data Sheet for CAS #68411-30-3 and in an analytical textbook.
Reference:	**81.** Cross, J. and Dekker, M (ed.). 1977. Anionic surfactants: chemical analysis. Vol.8. pp 111-115.
Reliability:	2 Valid with restrictions.

8.2.3 Theoretical Distribution Between Environmental Compartments (Fugacity Calculation)

CAS No. 68411-30-3

(a)

Media:	Air-biota [ ]; Air-biota-sediment-soil-water [X]; Soil-biota [ ]; Water-air [ ]; Water-biota [ ]; Water-soil [ ]
Method:	Fugacity level I and II Mackay-type modeling involving classifying the chemical and quantifying the emissions into each of five environmental compartments. The characteristics of the chemical are determined using a quantitative equilibrium criterion model (EQC). The EQC uses a generic, evaluative environment which is 100,000 km^2 in area. Estimated properties used as input parameters to the model are shown below: Molecular mass - 348 Air-water partition coefficient – 0 Aerosol-water partition coefficient – 100 Soil-water partition coefficient (L/kg) – 20 Sediment-water partition coefficient (L/kg) – 570 Fish-water partition coefficient (L/kg) – 250 Half life in air (h) – N/A Half life in water (h) – 24 Half life in soil (h) – 480 Half life in sediment (h) – 96

	The level I calculation assumes a steady-state equilibrium partitioning of a fixed quantity of LAS (100,000 kg) with no reaction or advection processes. The level II calculation assumes a fixed input of 100 kg/h, which is balanced by reaction and advection losses. Relative partitioning is identical to level I.
Results:	Level I and II models each resulted in LAS partitioning to air, water, soil and sediment at percentages of 0%, 25.97%, 56.09% and 17.76%, respectively. The overall residence time of LAS is 100 hours and removal is primarily by biodegradation (76%) and partitioning in sediment (13%).
Remarks:	This study was conducted by the model developer (an acknowledged expert on fugacity) to demonstrate the approach was appropriate for different types of chemicals. The discharge assumptions for LAS are noted to be highly conservative.
Reference:	**82.** Mackay, D, Di Guardo, A, Paterson, S, Kicsi, G, Cowan, C and Kane, D. 1996. Assessment of chemical fate in the environment using evaluative, regional and local scale models: Illustrative application to chlorobenzene and linear alkylbenzene sulfonates. Environ. Toxicol. Chem. 15:1638-1648.
Reliability:	1 Valid without restriction

8.2.4 Biodegradation

CAS No. 26264-05-1

(a)

Type:	aerobic **[ ]**; anaerobic **[ ]**
Medium:	water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Results:	This product is biodegradable
Method:	Not provided
Test substance:	Product contains 95% CAS No. **26264-05-1** (isopropylamine dodecylbenzene sulfonate) and 4% water.
Reference:	**40.** Material Safety Data Sheet for Bio-Soft N-411; 10/21/2004
Reliability:	4 Not assignable. Secondary literature.

CAS No. 27323-41-7

(a)

Type:	aerobic **[ ]**; anaerobic **[ ]**
Medium:	water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Results:	This product is biodegradable
Method:	Not provided
Test substance:	Product contains 55-65% CAS No. **27323-41-7** (triethanolamine dodecylbenzene sulfonate), 30-40% water, 2-2.5% sodium sulfate
Reference:	**41.** Material Safety Data Sheet for Bio-Soft N-300; 08/7/2007
Reliability:	4 Not assignable. Secondary literature.

(b)

Title The evaluation of the biodegradation of 910-92 using the OECD screening test method

Date of report July 2, 1986.

GLP Yes.

Reference **20. Pence W**.1986. The evaluation of the biodegradation of 910-92 using the OECD screening test method. Hill Top Research.

Test substance Benzenesulfonic acid, dodecyl-, compd. with 2,2',2"-nitrilotris(ethanol) (1:1));
Bio-Soft LD-190; Blend consists of 10% triethanolamine dodecyl benzene sulfonate (**CAS 27323-41-7**), 59% nonylfenol ethoxylate, 17% ether sulfate, 10% TEA, <5% cocamide DEA and <5% ethanol.

Test method EPA TSCA test guidelines 40 CFR 796.3240, Modified OECD screening test (1985).

Test system

Treatment
- Inoculum: prepared from soil (supernatant of aqueous suspension), secondary effluent from a sewage treatment plant and surface water (1:1:1). Each flask was inoculated with 0.5 mL of the mixed composite inoculum.
- 2 flasks treated (medium + inoculum + Bio-Soft LD-190 (20 mg C/L));
- 2 flasks positive control (medium + inoculum + sodium benzoate (20 mg C/L));
- 2 flasks blank control (medium + inoculum).

Procedure Aliquots of a stock solution of the test substance (tested conc. 20 mg C/L), mixed composite inoculum (0.5 mL) and nutrient solution (1 L) were mixed. The test mixtures were incubated at 21-23°C for 35 days. Aliquots were removed from each flask on day 0, 7, 14, 21, 27, 28 and 35 for DOC analyses.

Results

day	***% degradation [% of day 0 values]***	
	Bio-Soft LD-190	***sodium benzoate (reference substance)***
0	0	0
7	58	99
14	63	100
21	68	100
27	73	98
28	71	100
35	72	100

Conclusion Test substance is biodegradable. 71% degraded after 28 days, but did not reach 60% in 10-day window.

Rev. note 1. Test substance is a blend containing 10% of substance B. Because (1)

the resulting biodegradation (72%) is of the entire blend, (2) substance B is only 10% of the blend, and (3) the other components of the blend are known to be biodegradable, the biodegradation of substance B cannot be accurately estimated from this study.

Reliability 4 Not assignable. Test substance was a blend.

(c)

Type:	aerobic **[X]**; anaerobic **[ ]**
Medium:	water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[X]**
Results:	95%
Method:	OECD 301E
Test substance:	CAS No. **27323-41-7** (dodecylbenzenesulfonic acid, cmpd with 2,2',2"-nitrilotriethanol (1:1))
Reference:	**37.** European Commission. IUCLID Dataset. 2000. Unger Fabrikker A/S
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

CAS No. 68411-32-5

(a)

Title		Biotic degradation (modified Sturm test) Evaluation, in an aqueous medium, of the "ultimate" biodegredability of substances: 1736-1A, 1736-1B, 1736-1C, 1736-1D, 1736-1E
Date of report		Not indicated.
GLP		No data
Reference		**25. Stepan.** 1993. Biotic degradation (modified sturm test) evaluation, in an aqueous medium, of the "ultimate" biodegradability of substances: 1736-1A 1736-1B 1736-1C 1736-1D 1736-1E INERIS.
Test substance		1736-1E, purity 96%. Benzenesulfonic acid, dodecyl-, branched
Test method		OECD 301B.
Test system	**Design**	Two control flasks (medium + inoculum 30 mL), 2 treated flasks (medium + inoculum 30 mL + test substance 10 and 20 mg C/L), 1 flask for positive control (medium + inoculum 30 mL + aniline 20 mg C/L).
	Procedure	Incubation was performed in 5 L flasks containing 3000 mL of mineral solution with test substance and/or inoculum from activated sludge from a plant treating predominantly domestic sewage. The inoculum was treated and aerated for 28 days at 22±2°C with CO_2-free air in the dark. The outcoming air was passed through

CO_2-traps containing $Ba(OH)_2$. CO_2 was determined in the traps by back titration of residual $Ba(OH)_2$ after 1, 4, 5, 7, 8, 11, 12, 13, 15, 18, 20, 22, 26, 27 and 28 days. Samples of the incubate were removed on day 0 and 28 for DOC analysis.

Results **Analysis** DOC analysis: 94-107% of nominal (day 0); after 28 days: 14.4-17.2% of nominal was left for 1736-1E (82-87% degraded) and 0.3% of nominal for aniline (100% degraded).
For further results see table below.

	% biodegradation [% of $ThCO_2$] on day:														
Treatment	**1**	**4**	**5**	**7**	**8**	**11**	**12**	**13**	**15**	**18**	**20**	**22**	**26**	**27**	**28**
1736-1E (10 mg C/L)	1.6	15	28	41	48	56	61	62	64	66	68	70	71	72	73
1736-1E (20 mg C/L)	0.3	3.9	16	32	40	49	51	53	56	59	61	62	64	65	64
Positive control	0.0	19	41	58	64	72	76	78	80	83	86	87	89	89	89

Conclusion Biodegradable. 64-73% after 28-days at 10 mg/L and 20 mg/L, respectively. Meets the 10-day window for readily biodegradable at 10 mg/L but not at 20 mg/L.

Reliability 2 Reliable with restrictions.

CAS No. 68608-88-8

(a)

Type: aerobic **[ ]**; anaerobic **[ ]**
Medium: water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Results: This product is biodegradable
Method: Not provided
Test substance: Product contains >93% CAS No. **68608-88-8** (alkylbenzene sulfonic acid (C11-13) Br), <5.5% benzene, C10-16-alky derivs, and <1% sulphuric acid.
Reference: **38.** Material Safety Data Sheet for Ninate 411 Acid; 11/5/2004
Reliability: 4 Not assignable. Secondary literature.

CAS No. 68608-89-9

(a)

Type: aerobic **[ ]**; anaerobic **[ ]**
Medium: water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Results: This product is biodegradable
Method: Not provided
Test substance: Product contains 22% sodium dodeclybenzenesulfonate (C11-13 Br) CAS No. 68608-89-9, 74-78% water and <1% sodium sulphate and alkylbenzenesulfonic acid (C111-13 Br)
Remarks: none
Reference: **39.** MSDS for Polystep A-16-22 06/05/2006.
Reliability: 4 Not assignable. Secondary literature.

CAS No. 68411-30-3

(a)

Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	Bacterial biomass obtained from the settled supernatant slurry solution of a fertile soil
Concentration:	10 mg/L
Medium:	water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation:	See methods
Results:	See remarks
Method:	OECD 301E Ready Biodegradability test, with the following modifications: LAS was the sole source of carbon introduced (i.e., no activated sludge inoculum), along with an enriched level of bacterial biomass. Preliminary tests showed that more than 90% of the LAS disappeared within 4 days, so LAS was restored by adding about 10 mg/L of fresh substance every 4 days for 80 days. The test was stopped 4 days after the last LAS addition (i.e., at 84 days). Specific HPLC analysis was used to measure LAS and SPCs.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test Substance:	Commercial HF-type LAS with a C_{10}-$_{13}$ alkyl chain and a linearity of about 93% (DATS <0.5%; iso-branching 5-6%). (CAS #**68411-30-3**); average alkyl chain length = $C_{11.6}$
Remarks:	The final organic residue of this prolonged biodegradation test was characterized in detail and showed that no accumulation of iso-branching structures had occurred. This indicates that iso-branched material of LAS is amenable to biodegradation as well as the linear components.
Reference:	**44.** Cavalli, L., Cassani, G., Lazzarin, M., Maraschin, C., Nucci, G. and Valtorta, L. 1996b. Iso-branching of linear alkylbenzene sulphonate (LAS). Tenside Surf. Det. 33:393-398.
Reliability:	2 Valid with restrictions.

(b)

Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	adapted **[ ]**; non-adapted **[X]**; activated sludge, domestic
Concentration:	10.8 mg/L related to COD **[ ]**; DOC **[X]** test substance **[ ]**
Medium:	water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation:	93% after 28 days
Results:	readily biodeg. **[X];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Kinetic:	7 day = 59% 14 day = 73% 21 day = 82%
Method:	Directive 79/831/EEC, Appendix V, C.4-A 1990. DOC Die-Away Test. (OECD 301A Test). Samples were collected from an activated sludge basin with predominantly local municipal waste water. The final sludge concentration was 19.3 mg/L. Two

	replicates were used for the LAS test concentration (9.44 mg/L) with inoculum, one with inoculum without LAS, and two control replicates (sodium benzoate, 10.13 mg/L) with inoculum. A total of 900 mLs of the solutions were put into 2000 mL Erlenmeyer flasks at the beginning of the test. The loosely covered flasks were incubated at 21.5 to 22.6°C in the dark on a mechanical shaker for 28 days. Samples were collected on days 0, 7, 14, 21 and 28 for DOC analysis.
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	Marlon A 390 (CAS #**68411-30-3**) C_{10-13} LAS; average alkyl chain length = $C_{11.6}$
Remarks:	LAS is readily biodegradable. The 10-day window criterion was fulfilled. The control substance (sodium benzoate) showed 99% degradation after 28 days. This is a key study for ready biodegradability (see SIAR Table 4).
Reference:	**45.** Schoeberl, P. 1993b. Bestimmung der biologischen Abbaubarkeit von Marlon A 390 im DOC-DIE AWAY Test. Huels Final Report No. DDA-21.
Reliability:	1 Valid without restriction
(c)	
Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	adapted **[ ]**; non-adapted **[X]**; activated sludge
Concentration:	9.7 mg/L related to COD **[ ]**; DOC **[X]** test substance **[ ]**
Medium:	water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation:	94% after 28 days
Results:	readily biodeg. **[X];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Kinetic:	3 day = 38% 7 day = 81% 14 day = 88% 21 day = 94%
Method:	Directive 79/831/EEC, Appendix V, C.4-A - Year: 1990. DOC Die-Away Test. (OECD 301A Test). Samples were collected from an activated sludge basin with predominantly local municipal waste water. The final sludge concentration was 18.1 mg/L. Two replicates were used for the LAS test concentration (8.96 mg/L) with inoculum, one with inoculum without LAS, and two control replicates (sodium benzoate, 11.65 mg/L) with inoculum. A total of 900 mLs of the solutions were put into 2000 mL Erlenmeyer flasks at the beginning of the test. The loosely covered flasks were incubated at 21.8 to 22.2°C in the dark on a mechanical shaker for 28 days. Samples were collected on days 0, 3, 7, 14, 21, 27 and 28 for DOC analysis.
GLP:	Yes **[X]** No **[ ]** ? **[ ]**

Test substance:	Marlon A 390 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$
Remarks:	LAS is readily biodegradable. The 10-day window criterion was fulfilled. The control substance (sodium benzoate) showed 96% degradation after 28 days. This is a key study for ready biodegradability (see SIAR Table 4).
Reference:	**46.** Schoeberl, P. 1993. Bestimmung der biologischen Abbaubarkeit von Marlon A 390 im DOC-DIE AWAY Test. Huels Report No. DDA-32.
Reliability:	1 Valid without restriction

(d)

Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	adapted **[ ]**; non-adapted **[X]**; municipal sewage treatment plant effluent.
Concentration:	5 mg/L related to COD **[ ]**; DOC **[X]** test substance **[ ]**
Medium:	water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation:	76% after 28 day
Results:	readily biodeg. **[X];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Method:	Directive 84/449/EEC, C.3 Modified OECD screening test. (OECD 301E Test).
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$
Reference:	**47.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(e)

Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	adapted **[ ]**; non-adapted **[X]**; activated sludge
Concentration:	10 mg/L related to COD **[ ]**; DOC **[X]**; test substance **[ ]**
Medium:	water **[X]**; water-sediment **[ ]**; soil **[ ]**; sewage treatment **[ ]**
Degradation:	91.6% based on DOC reduction
Results:	readily biodeg. **[ ]**; inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[X]**
Method:	OECD Guideline 303 A "Simulation Test - Aerobic Sewage Treatment: Coupled Unit Test" 1981. The studies were carried out in the OECD Confirmatory Test plant at different laboratories using synthetic wastewater as specified in the EC Guidelines 82/242 and 82/243. The amount of surfactant supplied was 10 mg/ of MBAS/L. The amount of MBAS in the wastewater feed

corresponds approximately to that detected in the feed of municipal sewage plants, which corresponds to about 6 mg DOC/L. Test periods in the different laboratories ran from 33 to 139 days.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-13} LAS, sodium salt (CAS #**68411-30-3**); average alkyl chain length = $C_{11.6}$

Remarks: The degradation rate of 91.6% is the mean of 10 studies conducted at 7 different laboratories, based on DOC reduction. Since numerous studies have shown that not only anionic surfactants are shown in the MBAS analysis, the degradation plant discharge was analyzed on days 22, 24, 29 and 30 using HPLC analysis. Results showed that the content of intact LAS was < 20 µg/L, which is about 8% of the 250 µg/L MBAS content in the discharge. This means that the real LAS primary degradation reaches 99.8%.

Reference: **48.** Schoeberl, P. 1991. Coupling the OECD confirmatory test with continuous ecotoxicity tests. Tenside Surf. Det. 28:6-14.

Reliability: 2 Valid with restrictions

(f)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; municipal sewage treatment plant effluent

Concentration: 5 mg/L related to COD **[ ]**; DOC **[ ]**; test substance **[X]** MBAS

Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**

Degradation: 95% after 19 days

Results: readily biodeg. **[X];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**

Method: OECD Screening Test according to "Verordnung ueber die Abbaubarkeit anionischer und nichtionischer grenzflaechenaktiver Stoffe in Wasch- und Reinigungsmittel vom 30.1.1977". Bundesgesetzblatt Teil I, S. 244. 1977

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$

Reference: **47.** European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(g)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; synthetic sewage

Concentration: 19.2 mg/L related to COD **[ ]**; DOC **[ ]**; test substance **[X]**

Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**

Degradation:	92.3% based on DOC reduction
Results:	readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[X]**
Method:	OECD-Guideline 303A coupled units test. The studies were carried out in the OECD Confirmatory Test plant at different laboratories using synthetic wastewater as specified in the EC Guidelines 82/242 and 82/243. In these studies, LAS was added to the test at 10 mg/L. Test periods in the different laboratories ran from 33 to 139 days. Test temperature ranged from 19.6-23.0^{o}C.
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	Marlon A390 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.8}$
Remarks:	The degradation rate of 92.3% is the mean of 10 studies conducted at 7 different laboratories, based on DOC reduction, with LAS added to the confirmatory test plant.
Reference:	**48.** (1) Schoeberl, P. 1991. Coupling the OECD confirmatory test with continuous ecotoxicity tests. Tenside Surf. Det. 28:6-14. (2) European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	2 Valid with restrictions

(h)

Type:	aerobic **[X]**; anaerobic **[ ]**
Method:	Dialkyltetralin sulfonates (DATS) and LAS with single methyl branching on the alkyl chains (iso-LAS) are minor components in commercial LAS. In this study, DATS and iso-lAS were synthesized and exposed to simulated activated sludge, soil, and receiving water environments. In addition, the effluents coming from activated sludge treatment, which contained biodegradation intermediates, were exposed to simulated receiving water environments. Radiolabeled LAS, DATS and iso-LAS were used and all samples were analyzed using chemical-specific HPLC procedures. Surface soils were collected at three locations to represent "pristine" soil, sludge-amended soil, and gray water contaminated soil from the top of a percolation bed that receives surface applications of laundry water from a Laundromat. All samples were screened to remove vegetation, rocks and debris, and mixed with a mineral salts medium containing the test substance. Sediment samples were collected from the upper inch of a small stream that received effluent from a domestic wastewater treatment plant. Periphyton samples were collected as rocks coated with heavy growth from the same stream locations as the water and sediment samples. Each test system consisted of duplicate test flasks and a control flask. Tests lasted at least 30 days. For assessing biodegradation, the porous pot method was used in a

simulated wastewater activated sludge modified from ASTM test method E1798-96. A 21-day acclimation phase was followed by a 15-day test phase in which radioactivities in C02, liquids and solids, and effluent total suspended solids and COD were determined each day. Radiochemical recoveries for the porous pot test were calculated. For the die-away tests with porous pot effluents, the combined effluents from individual units were tested for mineralization of radiolabeled parent and intermediate compounds. All tests were run at least 30 days and the radioactivities measured at the end of each test.

Results: Results indicate that radiolabeled DATS and iso-LAS is mineralized by indigenous microbial populations in laboratory simulations of aquatic and soil environments. Half-lives ranged from 2 to 20 days. In addition, upon exposure to laboratory activated sludge treatment, most iso-LAS compounds showed >98% parent compound removal, extensive mineralization (>50%), and 79-90% ultimate biodegradation. Activated sludge treatment of DATS resulted in >98% removal, 3-12% ultimate biodegradation, and apparent formation of carboxylated biodegradation intermediates that accounted for 88-97% of the original material. These intermediatel continued to mineralize in simulated receiving water and soil environments at rates similar to that of sulfophenyl carboxylate (SPC) intermediates of a standard LAS.

Test Substances: ^{14}C-benzene ring labeled C_{12} LAS (97.5% radiochemical purity); ^{14}C-benzene ring labeled iso-LAS of the following types (IA, 97.8% purity; IB, 77.6% purity; IIA, 94.7% purity; IIB, 97.5% purity); ^{14}C-benzene ring labeled DATS (97.3% purity), plus the non-labeled versions of the same. ***Branched LAS***

Reference: **50.** Nielsen, A.M., Britton, L.N., Beall, C.E., McCormick, T.P. and Russell, G.L. 1997. Biodegradation of coproducts of commercial linear alkylbenzene sulfonate. Environ. Sci. Technol. 31:3397-3404.

Reliability: 2 Valid with restrictions

(i)

Type: aerobic **[X]**; anaerobic **[ ]**

Method: OECD 301E. The study was designed to investigate the biodegradation of a relatively high iso-branched form of commercial LAS. The test was a prolonged batch-biodegradation experiment in which the material is kept “alive” for 80 days and in which the test compound present in a mineral salts medium is the sole carbon source. An enriched level of bacterial biomass, three times the amount recommended, was added at the test start using an inoculum obtained from the settled supernatant slurry solution of a fertile soil, without any previous exposure to the test compound. LAS was maintained by adding about 0 mg/L of fresh substance

every four days for 80 days. After 80 days the test solution was sampled, centrifuged, sterilized with $HgCl_2$ solution and analyzed with a chemical specific HPLC method with fluorescence detection.

Results: Results indicate a residual LAS amount of 1.5 mg/L and SPC intermediate amount of 28.7 mg/L at the end of the 80 day study. Four distinct SPCs originating from the linear components of LAS were formed from the biodegradation experiment, and made up most of the organic residue. No evidence of structures related to the iso-branched material was found in the residue, therefore no accumulation of these materials is indicated. The iso-branched component of LAS and the corresponding SPCs mineralized at rates as fast as the linear components.

Test Substances: Commercial LAS (HF type) with a C_{10}-C_{13} alkyl chain and a linearity of about 93%, with a low DATS content (<0.5%) and a relatively high iso-LAS content (6.5%). ***Branched LAS***

Reference: **44.** Cavalli, L., Cassani, G., Lazzarin, M., Maraschin, C., Nucci, G., and Valtorta, L. 1996. Iso-branching of linear alkylbenzene sulphonate (LAS). Tenside Surf. Det. 33:393-398.

Reliability: 2 Valid with restrictions

(j)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; activated sludge

Concentration: 34.3 mg/L related to COD **[ ]**; DOC **[X]** test substance **[ ]**

Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**

Degradation: 85% after 29 days

Results: readily biodeg. **[X];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**

Kinetic:
0 day = -1%
2 day = -2%
5 day = 22%
9 day = 52%
12 day = 70%
14 day = 70%
21 day = 78%
28 day = 83%
29 day = 85%

Method: OECD Test Guideline 301B and EC Directive 92/69/EEC C.4-C. Modified Sturm Test.. The test substance was added to a defined liquid mineral medium which was inoclulated with an activated-sludge inoculum and aerated at 19.7-21.9°C (mean 21.1°C). The inoculum used was activated non-adapted sludge from the Marl-Ost municipal sewage treatment plant. The inoculum had a bacterial count of 81 x 10^4 CFU/mL as determined by the Koch pour-plate method. The CO_2 released was bound in the form of sodium carbonate in sodium hydroxide solution. Samples were collected

and analyzed in duplicate for bound CO_2 by TIC analysis after 0, 2, 5, 9, 12, 14, 21, 28 and 29 days. Sodium benzoate was used as a suitable control substance to monitor the activity of the inoculum. On the 29th day, residual dissolved CO_2 was expelled by acidification.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: Marlon A 365 WEL 6859 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; Activity: 65%

Remarks: LAS is readily biodegradable. The 10-day window criterion was fulfilled. The control substance (sodium benzoate) showed 89% degradation after 29 days. This is a key study for ready biodegradability (see SIAR Table 4).

Reference: **51.** Enste-Diefenbach, R.. 2002. Marlon A 365 WEL 6859: Determination of biodegradability in the modified Sturm test.. Infracor GmbH Analytical Tehcnical Services, Report ST-204/02.

Reliability: 1 Valid without restriction

(k)

Type: aerobic **[ ]**; anaerobic **[X]**

Methods: Experiments were conducted in which enriched cultures of anaerobic bacteria were provided with 60 μmole/L LAS as the sole source of sulfur. Conditions were maintained anoxic in salts-medium containing several sources of carbon.

Results: Strain RZ LAS, an anaerobic bacteria, was isolated from wastewater treatment plants in Germany. RZLAS was shown to degrade LAS, indicating that microorganisms able to metabolize LAS in anaerobic conditions exist in nature.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test Substance: Commercial C_{10-13} LAS (CAS #**68411-30-3**; average alkyl chain length = $C_{11.6}$) and C_{12} LAS (pure homologue)

Reference: **49.** Denger, K. and Cook, A.M. 1999. Linear alkylbenzene sulphonate (LAS) bioavailable to anaerobic bacteria as a source of sulphur. Journal of Applied Microbiology. 86:165-168.

Reliability: 2 Valid with restrictions

(l)

Type: aerobic **[ ]**; anaerobic **[X]**

Methods: Sediment cores and anoxic water samples were collected from a channel in Spain. Sediment slurries were prepared in an anaerobic chamber. LAS was added to obtain final concentrations of 10, 20 and 50 ppm. These microcosms were incubated at 30 C and several were sacrificed at days 0, 15, 60 and 165 days. Measurements included sulphide, methane, LAS, sulfophenyl carboxylic acid, and bacteria by cell count and DNA extractions,

Results: Degradation of LAS reached 79% in 165 days and generated sulfophenyl carboxylic acids (SPCA). The LAS was attached to the

	sediment, while the SPCAs were in solution. The average half life for LAS in these anoxic conditions was 90 days. High sulfate-reducing and methanogenic activities were recorded during the experiment and several bacterial strains were isolated.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test Substance:	Commercial LAS (CAS #**68411-30-3**)
Reference:	**91.** Lara-Martin, PA, A Gomez-Parra, T Kochling, J L Sanz, R Amils and E Gonziez-Mazo. 2007. Anaerobic Degradation of Linear Alkylbenzene Sulfonates in Coastal Marine Sediments. Environ. Sci. Technol. 41(10):3573-3579.
Reliability:	2 Valid with restrictions

8.2.5 Bioconcentration

CAS No. 42615-29-2

(a)

Title	Bioconcentration of linear alkylbenzene sulfonate (LAS) in bluegill *(Lepomis macrochirus)*
Date of report	1981.
GLP	No.
Reference	**8. Kimerle R., Macek K., Hasbrouch Sleight III, Burrows M.** 1981. Bioconcentration of linear alkylbenzene sulfonate (LAS) in bluegill (*Lepomis Macrochirus*). Wat. Res. 15: 251-256.
Test substance	Benzenesulphonic acid, linear alkyl, 14C-ring-labeled LAS.
Test method	Not specified.

Procedure Bluegill (*Lepomis macrochirus*), 4.0 g and 68 mm, were exposed to isotopically diluted ^{14}C-ring-labeled-LAS at mean measured concentration of 0.50 mg/L (SD 12%) for 21 days, followed by 14 days of depuration. The test included an untreated control and was conducted under flow-through (~20 changes/24 h) at 17±1°C, pH 7.1 in 60 L aquaria containing water of hardness 35 mg/L ($CaCO_3$). After equilibration of the test system (6 days), the control and the treatment were assigned to one tank each with initially 100 and 375 bluegills respectively (loading 12 and 3.2 L/fish/24 h). Fish were fed once daily and the O_2 was measured twice a week: O_2 >60%.
Four fish were removed for radiometric analysis on day 1, 3, 7, 11, 15 and 21 of uptake and on day 1, 2, 3, 5, 7, 9, 11 and 14 of depuration. On day 3, 16 and 21 of uptake and on day 1 and 3 of depuration 16 fish were removed for blood analysis. Water samples for radiometric analyses were taken at day 0, 1, 3, 7, 11, 15 and 21. The water samples were analysed by LSC. The fish for radiometric analysis were blotted dry, weighed and divided into gall bladder, liver, muscle with skin attached, visceral remains containing gills and esophagus and the remaining carcass with head, backbone, fins and tail and analysed by combustion/LSC.

Results The radioactivity (r.a.) concentration in the water was 100±12% (mean±SD). LOQ: 0.03 mg LAS/L.

Values for BCF, k_{uptake} and $k_{depuration}$, number of days to clear 50 and 90% of the steady state concentration (reached on day 7) were determined using the BIOFAC program.

Sample	*K_{uptake} (L/mg·d)*	*$K_{depuration}$ (d^{-1})*	*BCF (L/mg)*	*Days to reach 90% of steady state*	*Days to reach 50% of steady state*
Whole body	25 (8.0)[1]	0.24 (8.3)	104 (13)	9.7 (10)	2.9 (10)
Muscle (edible part)	9 (11)	0.24 (8.3)	36 (14)	9.4 (7.9)	2.8 (7.9)
Gall bladder	1461 (17)	0.28 (14)	5224 (22)	8.2 (13)	2.5 (14)
Liver	82 (26)	0.48 (8.3)	171 (29)	4.8 (85)	1.5 (8.3)
Gill and viscera	68 (12)	0.24 (13)	282 (17)	9.5 (12)	2.9 (12)
Blood	62 (1.6)	0.26 (3.8)	237 (2.5)	8.7 (1.4)	2.6 (0.4)
Remaining carcass	15 (13)	0.24 (8.3)	64 (14)	9.7 (9.4)	2.9 (9.3)

[1] ( ) Standard deviation (%)

Conclusion Whole fish: steady state uptake reached after 7 days; BCF (based on r.a.) 104; DT_{50} depuration r.a. 2.9 day, DT_{90} depuration r.a. 9.7 day.

Rev. note
1. Since no results of spiked water or spiked fish were included, the validity of the analytical methods cannot be checked.
2. The calculated BCF values are based on total radioactivity. The

rapid elimination of LAS, suggests metabolic deactivation. The BCF based on radioactivity is presumably an overestimation of that based on parent.

Reliability **2** Valid with Restrictions. No QC analytic samples were included (note 1).

CAS No. 68411-30-3

(a)

Species:	*Lepomis macrochirus*
Exposure Period:	21 days
Temperature:	$17^{+}/-1^{o}C$
Concentration:	0.5 mg/L
BCF:	104 (whole body); 36 (muscle)
Elimination:	Yes
Method:	Bluegill sunfish (avg wt. 4.0 g; avg length 68 mm) were placed in a 60 liter aquarium (375 fish total) and maintained for 21 days. A second aquarium held 100 control fish. Fish were fed daily with a dry pelleted trout chow ration of approximately 2% of body weight. Water samples were removed periodically for radiometric analysis of ^{14}C-labeled LAS. Four fish were removed on each of days 1, 2, 3, 5, 7, 9, 11 and 14 for radiometric analysis.
Type of test:	calculated **[ ]**; measured **[ ];** static **[ ]**; semi-static **[ ]**; flow-through **[X]**
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{10-13} LAS (CAS #**68411-30-3**) with the following alkyl chain length distribution: C_{11} 45%, C_{12} 36.5%, C_{13} 18.5%. Average chain length was 11.7 and molecular weight was 344.
Remarks:	The site of greatest concentration was the gall bladder with a BCF of 5000, based on total radiolabeled materials. The BCFs for liver, gills and viscera, remaining carcass, and blood ranged from 64 to 283. Clearance of radiolabeled materials was rapid with half-lives of 2 to 5 days. However, no quantitative conclusions specific to LAS can be drawn from these data, as total radiolabeled materials were measured, and these likely include LAS metabolites.
Reference:	**8.** Kimerle, R.A., Macek, K.J., Sleight, B.H. and Burrows, M.E. 1981. Bioconcentration of linear alkylbenzene sulfonate (LAS) in bluegill (*Lepomis macrochirus*). Wat. Res. 15:251-256.
Reliability:	2 Valid with restrictions

8.3 Ecotoxicity Endpoints

8.3.1 Acute/Prolonged Toxicity to Fish

CAS No. 26264-05-1

(a)

Title Static acute toxicity of CASRN 26264-05-1 to the fathead minnow (*Pimephales promelas*)

Date of report April 27, 2000.

GLP No.

Reference **10. Kuc W.** 2000. Static acute toxicity of CASNR 26264-05-1 to Fathead minnow (*Pimephales promelas*). Baker Petrolite.

Test substance Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1)), purity 89.4%

Guideline OECD 203.

Stat. method None

Test system

Species Fathead minnow (*Pimephales promelas)*, mean length 17 mm.

No. of fish 10/replicate, 2 replicates/treatment.

Concentrations Nominal: 3.2, 5.6, 10, 18, 32 and 56 mg/L, water treated controls.

Test conditions Static; at 20±2°C in 21 L glass-silicone vessels containing 10 L reconstituted water (pH 8.3, hardness 168 mg/L $CaCO_3$); 16 h light; unfed, loading 0.04 g/l.

Phys. meas. Daily in all treatments: overall ranges for pH 8.2-8.4; O_2 87-100%; temperature 20-22°C.

Observations Mortality/symptoms at 24, 48, 72 and 96 h.

Results

		Nominal concentration [mg/L]						
Parameter	**Time [h]**	**0**	**3.2**	**5.6**	**10**	**18**	**32**	**56**
Mortality [%]	96	0	5	0	0	15	100	100
Symptoms*	24-96					+		

*Symptoms included twitching, quiescent, dark discolored, gulping air and/or labored.

Conclusion The 96-h LC_{50} calculated by the author using trimmed SPK was 22 mg/L (95% CI 20-24 mg/L) ⇔ 20 mg a.i./L (95% CI 18-22 mg/L).

Reliability 2 Valid with restrictions. Static test with no chemical analyses performed; non-GLP study.

(b)

Results: 96-hr fish LC50 = 2.6 mg/L

Method: Estimated by Calculation

GLP: Not applicable

Test Substance: **26264-05-1.** Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1)

Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 27323-41-7

(a)

Species:	not indicated
Results:	LC_{50} values for fish: 1-5 mg/L
Test Substance:	CAS #**27323-41-7**
Remarks:	none
Reference:	European Commission. IUCLID Dataset for dodecyl benzenesulphonic acid, compound with 2,2',2"-nitrilotriethanol (1:1); CAS No. 27323-41-7. 18-FEB-2000. Unger FAbrikker A/S Fredrikstad.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Results:	96-hr fish LC50 = 2.6 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**27323-41-7.** dodecyl benzenesulphonic acid, compound with 2,2',2"-nitrilotriethanol (1:1) (1:1)
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 26264-06-2

(a)

Results:	96-hr fish LC50 = 2.6 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**26264-06-2.** benzenesulphonic acid, dodecyl, calcium salt
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68411-32-5

(a)

Results:	96-hr fish LC50 = 2.9 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68411-32-5.** benzenesulphonic acid, dodecyl, branched
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C11.9
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68953-96-8

(a)

Results:	96-hr fish LC50 = 0.46 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68953-96-8.** benzenesulphonic acid, mono-C11-13-branched alkyl derives., calcium salts
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C13.5
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68608-88-8

(a)

Results:	96-hr fish LC50 = 3.5 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68608-88-8.** benzenesulphonic acid, mono-C11-13-branched alkyl derives.
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C11.8
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 90218-35-2

(a)

Results:	96-hr fish LC50 = 3.5 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**90218-35-2.** benzenesulphonic acid, dodecyl-, branched, compds with 2-propanamine

Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C11.8
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68608-89-9

(a)

Results:	96-hr fish LC50 = 0.46 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68608-89-9.** benzenesulphonic acid, mono-C11-13-branched alkyl derives., sodium salts
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C13.5
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 42615-29-2

(a)

Title	Toxicity of a linear alkylate sulfonate detergent to larvae of four species of freshwater fish	
Date of report	1975.	
GLP	No data	
Reference	**14. McKim J., Arthur J., Thorslund T. 1975.** Toxicity of a linear alkylate sulfonate detergent to larvae of four species of freshwater fish. Bull. Environ. Contam. Toxicol. 14(1): 1-7.	
Test substance	Benzenesulphonic acid, linear alkyl; commercial detergent formulation containing 14% LAS; 2.3% alcoholethoxylate oxide condensate; 2.5% sodium soap; 48% sodium tripolyphosphate; 9.7% sodium silicate; 15.4% sodium sulphate; 8.1% moisture and miscellaneous.	
Guideline	Not indicated.	
Stat. method	One-way analysis of variance (Dunnett 1955).	
Test system	**Species**	Northern pike (*Esox lucius*); White sucker (*Catostomus commersoni*); Smallmouth bass (*Micropterus dolomieu*); Fathead minnow (*Pimephales promelas*): 2-3 days after hatching.
	No. of fish	50/test vessel (2 vessel/treatment) for Northern pike and White sucker; 25/test vessel (2 vessel/treatment) for Smallmouth bass; 15/test vessel (2 vessel/treatment) for Fathead minnow.
	Concentrations	0.2-0.3, 0.5, 1.1-1.2, 2.3-2.6 and 5.0-6.3 mg/L

MBAS (apprx. equivalent to LAS); untreated controls.

Test conditions 30-day flow-through (no aeration) in tanks containing 12.5 L of lake water (hardness 36-48 mg/L as $CaCO_3$), 6 replacements/24 h, temperature 15±1°C, except for *Pimephales promelas* 23±1°C; feeding at least twice daily.

Analysis Once a week for all concentrations (composite of daily taken samples) using the MBAS-procedure after preservation with 1% formaldehyde (ref. standard 4.045% aqueous LAS).

Phys. meas. One tank per week: overall ranges for pH 7.2-7.9; overall ranges O_2 5.6-10 mg/L.

Observations Mortality; body weight (total = standing crop) on day 30.

Results For analytical results see 1st table below. Biological data are shown in the 2nd table. QCs were completely recoverable.

Analysis

Test chamber	**Measured concentration ± standard error (mg/L)**			
	E. lucius	***C. commersoni***	***M. dolomieu***	***P. promelas***
1	5.9 ± 0.2	5.0 ± 0.3	6.3 ± 0.05	5.8 ± 0.35
2	2.4 ± 0.1	2.6 ± 0.15	2.5 ± 0.05	2.3 ± 0.05
3	1.2 ± 0.05	1.1 ± 0.10	1.2 ± 0.05	1.2 ± 0.05
4	0.5 ± 0.05	0.5 ± 0.05	0.5 ± 0.05	0.5 ± 0.01
5	0.3 ± 0.01	0.2 ± 0.01	0.3 ± 0.01	0.2 ± 0.05
Control	0.02 ± 0.005	0.01 ± 0.005	0.02 ± 0.005	0.02 ± 0.01

Biological

Parameter	**Time [d]**	**Mean measured concentration [mg/L]**					
		0	**0.2-0.3**	**0.5**	**1.1-1.2**	**2.3-2.6**	**5.0-6.3**
Standing crop* *E. lucius*	30		I	i	dc	dc	-
Standing crop *C. commersoni*	30		Dc	dc	dc	dc	dc
Standing crop *M. dolomieu*	30		Ic	ic	ic	Ic	dc
Standing crop *P. promelas*	30		=	d	dc	dc	-

* Standing crop: the biomass of a particular area, ecosystem etc. at any specified time.
d=decrease, I=increase, c=significant

Conclusions *Esox lucius* : 96-h LC50 3.7 mg/L; 30-d NOEC 0.6 mg/L
Catostomus commersoni : 96-h LC50 4.0 mg/L;
30-d NOEC ~0.2 mg/L
Micropterus dolomieu: 96-h LC50 3.7 mg/L;
30-d NOEC 3 mg/L
Pimephales promelas : 96-h LC50 3.4 mg/L;

30-d NOEC 0.5 mg/L

30-day NOEC based on standing crop

Rev. note
1. Because the test substance is a formulation, the observed toxicity reflects exposure to LAS and the other components. Nominal concentrations were not reported, so mean measured concentrations have been used in this summary. From the report it is not completely clear whether concentrations are expressed in mg formulation or mg active ingredient. It is assumed that concentrations are expressed in mg active ingredient (i.e., LAS) and this is consistent with the MBAS analytical measurement.
2. Observations were made for the dead of juvenile fish, but mortality is not reported. The LC50 values included in the conclusions could not be checked with the original data.

Reliability 2 Valid with restrictions. Incomplete description (notes 1 & 2).

(b)

Results:	96-hr fish LC50 = 2.6 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**42615-29-2.** benzenesulphonic acid, linear alkyl
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68584-26-9

(a)

Results:	96-hr fish LC50 = 0.75 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68584-26-9.** benzenesulphonic acid, C10-16-alkyl derives., magnesium salt
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C13
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 70528-83-5

(a)

Results:	96-hr fish LC50 = 1.3 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable

Test Substance: **70528-83-5.** benzenesulphonic acid, dodecyl-, branched, calcium salts

Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12.5

Reference: **89.** USEPA. ECOSAR version 0.99h (2007)

Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68411-30-3

(a)

Species: *Lepomis macrochirus* and *Pimephales promelas*

Results: LC_{50} values ranged from 1.67 to 7.7 mg/L for *L. macrochirus* (10 records) LC_{50} value for *P. promelas* = 4.1 mg/L (1 record).

Test Substance: $C_{10\text{-}13}$ LAS (CAS #**68411-30-3**)

Remarks: A total of 18 fish studies for these two species were reviewed by HERA in 2004. Seven of these studies were rejected because the test material was not commercial LAS, the study deviated significantly from standard protocols, or non-standard endpoints were measured. The remaining eleven studies were evaluated for reliability and the results reflect the range of acute LC_{50} values obtained for the most commonly tested fish species. These studies are tabulated and discussed further in the SIAR and SIAP in a weight-of-evidence approach. A robust summary for the study with the lowest LC_{50} value was prepared (see Lewis and Perry 1981 above).

Reference: **42.** HERA. 2004. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. **68411-30-3**, Version 2.0 June 2004. http://www.heraproject.com/riskassessment.cfm.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other**[ ]**
open-system **[X]**; closed-system **[ ]**

Species: *Brachydanio rerio* (Fish, fresh water)

Exposure period: 96 hour

Results: LC_{50} = 5.1 mg/L

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: OECD Guide-line 203 “Fish, Acute Toxicity Test”

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: $C_{10\text{-}13}$ LAS (CAS #**68411-30-3**)

Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. The submitter (Huels AG) judged the study quality to be good.

Water hardness: 310 mg/L $CaCO_3$; tap water diluent; 25 ºC; adult fish tested.

Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, AT/FU/80/90.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(c)

Type of test: static **[ ]**; semi-static **[X]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**

Species: *Brachydanio rerio* (Fish, fresh water)

Exposure period: 96 hour

Results: LC_{50} = 7.8 mg/L

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: ISO 7346/1-3

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = 11.6

Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Concentration of test substance related to MBAS. LC_0 and LC_{100} = 5.6 and 11 mg/L, respectively

Reference: **47.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(d)

Type of test: static [ ]; semi-static **[X]**; flow-through **[ ]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**

Species: *Salmo gairdneri* (Fish, estuary, fresh water)

Exposure period: 96 hour

Results: LC_{50} = 5.8 mg/L

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: OECD Guide-line 203 “Fish, Acute Toxicity Test”

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: C_{10-13} LAS (CAS # **68411-30-3**)

Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. The submitter (Huels AG) judged the study quality to be good. Analysis showed 92% of nominal concentration. Tap water diluent; water hardness = 96-120 mg/L $CaCO_3$; pH 6.8-7.3; daily renewal; 14.5-16ºC; 5 month old fish tested.

Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, AT/17.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(e)

Type of test: static **[ ]**; semi-static **[X]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**

Species: *Salmo gairdneri* (Fish, estuary, fresh water)

Exposure period: 96 hour

Results: LC_{50} = 3 mg/L

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: See remarks.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: DOBANIC ACID 102, C_{10-13} LAS (CAS #**68411-30-3**)

Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Daily renewal of test solutions; 14-16 ºC; pH 7.6-8.4; water hardness = 210-240 mg/L $CaCO_3$; DO=10.0-10.4
mg/L. Fingerlings were tested, mean weight 5.2 g

Reference: **53.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Shell Research Ltd, SBGR.81.083, RR Stephenson.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(f)

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**

Species: *Lepomis macrochirus* (Fish, fresh water)

Exposure period: 96 hour

Results: LC_{50} = 5.0 mg/L (mean of 8 tests)

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: EPA-660/3-75-009

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: C_{10-13} LAS, average chain length 11.8 (CAS #**68411-30-3**)

Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. LC_{50} values for the 8 tests conducted ranged from 3.7 to 7.7 mg/L. Nominal concentration, (expected deviation <20%), reconstituted water, water hardness = 30-48 mg/L CaCO3; pH 7.3-7.8; 20-23ºC; fish size: 0.35-0.89 g

Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing

Procter & Gamble, 1991, 22852, 23613, 23612, 23617, 23722, 22824, 28661, 27917.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(g)

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**

Species: *Lepomis macrochirus* (Fish, fresh water)

Exposure period: 96 hour

Results: LC_{50} = 2.2 mg/L

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: EPA-660/3-75-009

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: $C_{10\text{-}13}$ LAS, average chain length 11.8 (CAS #68411-30-3)

Remarks: Information as cited in IUCLID Data Sheet for CAS #**68411-30-3**. Huels AG judged study quality to be good. Nominal concentrations, (expected deviation <20%). Reconstituted water with hardness = 44 mg/L $CaCO_3$; pH 7.58; 22ºC; fish size: 0.35 g, 40 mm; Note that this study was not included in the HERA LAS acute toxicity data summary tables in the SIAR because only a summary of the study, not the full report, is available.

Reference: **52.** European Commission. 2000. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 22581, 28361.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(h)

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]** not stated

Species: *Pimephales promelas* (Fish, fresh water)

Exposure period: 96 hour

Results: LC_{50} = 4.6 mg/L

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: Ten fathead minnows were exposed for 96 hours to LAS under the following conditions: hardness 35 mg/L as $CaCO_3$; pH 7.1; temperature 21^{o}C. Fish were not fed during the exposure.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Low molecular weight LAS, sodium salt (CAS #**68411-30-3**); C_{10} 5%, C_{11} 27%, C_{12} 53%, C_{13} 13%, 2-phenyl 23%; average alkyl chain length = $C_{11.1}$.

Remarks: The carboxylated intermediates formed in the biodegradation of LAS were also tested and found to be several orders of magnitude less toxic than LAS. These intermediates undergo further

biodegradation, more rapidly in a natural river water than in a synthetic medium.

Reference **54.** Swisher, R.D, Gledhill, W.E, Kimerle, R.A. and Taulli, T.A. 1978 Carboxylated intermediates in the biodegradation of linear alkylbenzene sulfonates (LAS). VII International Congress on Surface Active Substances, Proceedings, Moscow, 1976 4:218-230.

Reliability: 2 Valid with restrictions

(i)

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**

Species: *Pimephales promelas* (Fish, fresh water)

Exposure period: 96 hour

Results: LC_{50} = 4.1 mg/L

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: USEPA methods for acute toxicity tests with fish, macroinvertebrates, and amphibians. Ecol. Res. Series. EPA-660/3-75-009.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-13} LAS, average chain length 11.7 (CAS #**68411-30-3**) (C_{10} 7.3%; C_{11} 26.5%; C_{12} 56.7%; C_{13} 9.0%; C_{14} 0.5%); Mean phenyl position = 3.9; Mean molecular weight = 345.

Remarks: Acute tests were conducted at EG&G Bionomics from 1971 to 1976 with 2-3 month old fathead minnows in 20-L glass vessels with soft reconstituted water (hardness = 40 mg/L as $CaCO_3$). Tests with LASs of average alkyl chain length of 11.2 and 13.3 were conducted concurrently, with the resultant 96 hour LC_{50} values of 12.3 and 0.86 mg/L, respectively.

Reference: **55.** Holman, W.F. and Macek, K.J. 1980. An aquatic safety assessment of linear alkylbenzene sulphonate (LAS); chronic effects on fathead minnows. Trans. Am. Fish. Soc. 109(1):122-131.

Reliability: 2 Valid with restrictions

(j)

Results: 96-hr fish LC50 = 2.6 mg/L

Method: Estimated by Calculation

GLP: Not applicable

Test Substance: **68411-30-3.** benzenesulphonic acid, C10-13 alkyl derives., sodium salt

Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12

Reference: **89.** USEPA. ECOSAR version 0.99h (2007)

Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 27176-87-0

(a)

Type of test:	static **[**X**]**; semi-static **[ ]**; flow-through **[ ]**; other**[ ]**
Species:	*Leuciscus idus* (Fish, fresh water)
Exposure period:	96 hour
Results:	LC_{50} = 4.1 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[]**
Method:	other: DIN 38412 Part 15
GLP:	Yes **[X]** No **[ ]** ? **[]**
Test substance:	benzene sulfonic acid, dodecyl- (**CAS # 27172-87-0**)
Remarks:	LC0 = 4, LC100 = 4.3
Reference:	**77.** Knie, VJ, Halke A, Juhnke, I and Schiller,W. 1983. Ergebnisse der untersuchungen von chemischen soffen mit vier biotests. Deutsch Gewasserkundliche Mitteilungen. 77-79.
Reliability:	1 Valid without restriction.

(b)

Type of test:	static **[]**; semi-static **[ ]**; flow-through **[ ]**; other**[X]** daily renewal
Species:	*Salmo gairdneri* (Fish, fresh water)
Exposure period:	96 hour
Results:	LC_{50} = 4.3 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[]**
Method:	OECD Guideline 203 “Fish acute toxicity test”
GLP:	Yes **[]** No **[X]** ? **[]**
Test substance:	benzene sulfonic acid, dodecyl- (**CAS # 27172-87-0**)
Remarks:	LC50 is geometric mean of lower (3.2 mg/L) and upper (5.6 mg/L) limits from a series of studies investigating the reduction in number of individuals needed for testing.
Reference:	**78.** Douglas, MT, Chanter, DO, Pell, IB and Burney, GM. 1986. A proposal for the reduction of animal numbers required for the acute toxicity to fish test (LC50 determination). Aquat. Toxicol. 8:243-249.
Reliability:	1 Valid without restriction.

(c)

Results:	96-hr fish LC50 = 2.6 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**27176-87-0.** benzenesulphonic acid, dodecyl
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

8.3.2 Acute Toxicity to Aquatic Invertebrates

8.3.2.1 Daphnia

CAS No. 26264-05-1

(a)

Title	Static acute toxicity of CASRN 26264-05-1 to *Daphnia magna*	
Date of report	May 8, 2000.	
GLP	No.	
Reference	**24. Steevens M.** 2000**.** Static acute toxicity of CASNR 26264-05-1 to Daphnia magna. Baker Petrolite.	
Test substance	Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1)), purity 89.4%.	
Test method	OECD 202.	
Stat. method	None.	
Test system	**Species**	*Daphnia magna*, <24 h old.
	No. of daphnids	5/replicate, 4 replicates/treatment.
	Concentrations	Nominal: 1.56, 3.13, 6.25, 12.5, 25, 50 and 100 mg/L (no vehicle), untreated controls.
	Test conditions	Static; at 20±2°C in 225 mL crystallising dishes (covered), containing 100 mL of reconstituted water of hardness 168 mg/l ($CaCO_3$) and pH 8.3, 16 h light.
	Phys. meas.	At 0 and 48 h in one replicate for all concentrations; overall ranges for pH 8.4-8.5; O_2 91-97%; temperature (0, 24 and 48 h) 20-21°C.
	Observations	Immobility/mortality at 24 and 48 h.

Results ***8.3.2.1.1.1.1***

		Nominal concentration [mg/L]							
Parameter	**Time [h]**	**0**	**1.56**	**3.13**	**6.25**	**12.5**	**25**	**50**	**100**
Immobility [%]	48	0	0	85	100	100	100	100	100

Conclusion The 48-h EC_{50} calculated by the author using trimmed SPK was 2.5 mg/L (95% CI 2.2-2.7 mg/L) ⇔ 2.2 mg a.i./L (95% CI 2.0-2.4 mg a.i./L).

Reliability Score 2 Valid with restrictions. Static test with no chemical analyses were performed; non-GLP study.

(b)

Results:	48-hr daphnid EC50 = 2.6 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**26264-05-1.** Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1)

Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 27323-41-7

(a)

Species:	*Daphnia magna*
Results:	LC_{50} = 15 mg/L
Test Substance:	CAS #**27323-41-7**
Remarks:	none
Reference:	**37.** European Commission. 2000. IUCLID Dataset for dodecylbenzenesulphonic acid, compound with 2,2',2"-nitrilotriethanol (1:1); CAS No. 27323-41-7. 18-FEB-2000. Unger FAbrikker A/S Fredrikstad.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Results:	48-hr daphnia EC50 = 2.6 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**27323-41-7.** dodecyl benzenesulphonic acid, compound with 2,2',2"-nitrilotriethanol (1:1)
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 26264-06-2

(a)

Results:	48-hr daphnia EC50 = 2.6 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**26264-06-2.** benzenesulphonic acid, dodecyl, calcium salt
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68411-32-5

(a)

Results:	48-hr daphnia EC50 = 2.9 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68411-32-5.** benzenesulphonic acid, dodecyl, branched
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C11.9
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68953-96-8

(a)

Results:	48-hr daphnia EC50 = 0.46 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68953-96-8.** benzenesulphonic acid, mono-C11-13-branched alkyl derives., calcium salts
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C13.5
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68608-88-8

(a)

Results:	48-hr daphnia EC50 = 3.5 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68608-88-8.** benzenesulphonic acid, mono-C11-13-branched alkyl derives.
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C11.8
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 90218-35-2

(a)

Results:	48-hr daphnia EC50 = 3.5 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**90218-35-2.** benzenesulphonic acid, dodecyl-, branched, compds with 2-propanamine

Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C11.8
Reference: **89.** USEPA. ECOSAR version 0.99h (2007)
Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68608-89-9
(a)
Results: 48-hr daphnia EC50 = 0.46 mg/L
Method: Estimated by Calculation
GLP: Not applicable
Test Substance: **68608-89-9.** benzenesulphonic acid, mono-C11-13-branched alkyl derives., sodium salts
Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C13.5
Reference: **89.** USEPA. ECOSAR version 0.99h (2007)
Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 42615-29-2
(a)
Results: 48-hr daphnia EC50 = 2.6 mg/L
Method: Estimated by Calculation
GLP: Not applicable
Test Substance: **42615-29-2.** benzenesulphonic acid, linear alkyl
Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference: **89.** USEPA. ECOSAR version 0.99h (2007)
Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68584-26-9
(a)
Results: 48-hr daphnia EC50 = 0.75 mg/L
Method: Estimated by Calculation
GLP: Not applicable
Test Substance: **68584-26-9.** benzenesulphonic acid, C10-16-alkyl derives., magnesium salt
Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C13
Reference: **89.** USEPA. ECOSAR version 0.99h (2007)
Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 70528-83-5

(a)

Results:	48-hr daphnia EC50 = 1.3 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**70528-83-5.** benzenesulphonic acid, dodecyl-, branched, calcium salts
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12.5
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68411-30-3

(a)

Species:	*Daphnia magna*
Results:	EC_{50} values ranged from 1.62 to 9.3 mg/L
Test Substance:	$C_{10\text{-}13}$ LAS (CAS #**68411-30-3**)
Remarks:	A total of 20 daphnid studies were reviewed by HERA in 2004. Nine of these studies were rejected because the test material was not commercial LAS, the study deviated significantly from standard protocols, or non-standard endpoints were measured. The remaining 11 studies were evaluated for reliability and the results reflect the range of acute EC_{50} values obtained for *Daphnia magna*. These studies are tabulated and discussed further in the SIAR and SIAP in a weight-of-evidence approach. A robust summary for the study with the lowest acute EC_{50} value was prepared (see Hooftman and van Drongelen-Sevenhuijsen above).
Reference:	**42.** HERA. 2004. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. **68411-30-3**, Version 2.0 June 2004. http://www.heraproject.com/riskassessment.cfm.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[ ]**; closed-system **[ ]** not stated
Species:	*Daphnia magna* (Crustacea)
Exposure period:	48 hour
Results:	EC_{50} = 6.8 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	Directive 84/449/EEC, C.2 “Acute toxicity for *Daphnia*” 1984
GLP:	Yes **[X]** No **[ ]** ? **[ ]**

Test substance: C_{10-13} LAS, sodium salt (CAS #**68411-30-3)**
Remarks: Information cited in IUCLID Data Sheet for CAS #68411-30-3.
Reference: **43.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Huels Study (unpublished).
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(c)
Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species: *Daphnia magna* (Crustacea)
Exposure period: 48 hour
Results: LC_{50} = 5.5 mg/L (mean of 3 valid tests)
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: EPA-660/3-75-009
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{10-13} LAS, average chain length 11.8 (CAS #**68411-30-3**)
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Life-stage: <24 h. Effect: immobility. LC_{50} values for 4 tests ranged from 4.4 to 10.4 mg/L. Huels AG judged study quality to be good. Nominal concentrations (expected deviation <20%). Reconstituted water with hardness = 162-220 mg/L $CaCO_3$. Note that all four of these studies are included in Appendix 2, the HERA acute toxicity data review. Three of the studies, Reports 23618, 22853 and 23611 with respective values of 4.4, 4.9 and 7.1 mg/L, are considered reliable and are included in the table of acute toxicity values. The fourth study, Report 23276 with a value of 10.4 mg/L, is listed among the rejected studies because it was conducted as part of a QA program to qualify various labs and the result is not considered reliable.
pH 7.86-8.53. 21-22ºC
Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 23618, 22853, 23611, 23276.
Reliability: 2 Valid with restrictions for the three valid studies. The original studies were reviewed by HERA (2004) for Annex 2.

(d)
Results: 48-hr daphnia EC50 = 2.6 mg/L
Method: Estimated by Calculation
GLP: Not applicable
Test Substance: **68411-30-3.** benzenesulphonic acid, C10-13 alkyl derives.,

	sodium salt
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 2**7176-87-0**

(a)

Species:	*Daphnia magna*
Results:	24-hr EC_{50} = 12 mg/L
Test Substance:	benzene sulfonic acid, dodecyl- **CAS #27176-87-0**
Remarks:	method was DIN 38412 Par 11; done under GLP; no analytical monitoring
Reference:	**77.** Knie, VJ, Halke A, Juhnke, I and Schiller,W. 1983. Ergebnisse der untersuchungen von chemischen soffen mit vier biotests. Deutsch Gewasserkundliche Mitteilungen. 77-79.
Reliability:	2 valid with restrictions. 24 hours is not the standard duration.

(b)

Species:	*Daphnia magna*
Results:	48-hr EC_{50} = 5.88 mg/L
Test Substance:	benzene sulfonic acid, dodecyl- **CAS #27176-87-0**
Remarks:	method was Directive 84/449/EEC, C.2 “Acute toxicity for Daphnia”; GLP not indicated; analytical monitoring performed
Reference:	**79.** European Commission. 1992. IUCLID dataset for benzene sulfonic acid, dodecyl- **CAS #27176-87-0**. 1995. cited Galassi et al. 1992. Water Research 26:19-27.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(c)

Results:	48-hr daphnia EC50 = 2.6 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**27176-87-0.** benzenesulphonic acid, dodecyl
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**89.** USEPA. ECOSAR version 0.99h (2007)
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

8.3.2.2 Other aquatic invertebrates

CAS No. 68411-30-3

(a)

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**

Species: *Chironomus riparius* (chironomid)

Exposure period: 96 hour

Results: LC_{50} = 6.5 mg/L

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: EPA

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: C_{10-13} LAS, average chain length 12.3 (CAS #**68411-30-3**)

Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Nominal concentrations (expected deviation <20%). Well water with hardness = 24-30 mg/L $CaCO_3$; pH 7.1; 21-22ºC

Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 34845.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**

Species: *Limnodrilus hoffmeisteri* (aquatic worm)

Exposure period: 96 hour

Results: LC_{50} = 1.8 mg/L

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: EPA 660/3-75-009

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: C_{10-13} LAS, average chain length 12.3 (CAS #**68411-30-3**)

Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Additional LC_{50} values for extended exposure times: 144 h: 1.1 mg/L, 196 h: 0.96 mg/L. Huels AG judged study quality to be good. Nominal concentrations (expected deviation <20%). Well water with hardness = 24-30 mg/L $CaCO_3$; pH 7.1; 21-22ºC.

Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 34845.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(c)

Type of test:	static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:	*Planaria* sp. (aquatic worm)
Exposure period:	48 hour
Results:	LC_{50} = 1.8 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	EPA 660/3-75-009
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	$C_{10\text{-}13}$ LAS, average chain length 12 (CAS #**68411-30-3**)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Nominal concentrations (expected deviation <20%). Reconstituted water with hardness 165 mg/L $CaCo_3$. pH 8.1–8.4; 21-22^oC; size 3.4 cm.
Reference:	**52.** European Commission. 2000. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 31340.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.3.3 Toxicity to Aquatic Plants (e.g., algae)

CAS No. 26264-05-1

(a)

Results:	96-hr algae EC50 = 70 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**26264-05-1.** Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1)
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 27323-41-7

(a)

Species:	not indicated
Results:	EC_{50} values for algae: 11-300 mg/L
Test Substance:	CAS #**27323-41-7**
Remarks:	none
Reference:	**37.** European Commission. 2000. IUCLID Dataset for dodecylbenzenesulphonic acid, compound with 2,2',2"-nitrilotriethanol (1:1); CAS No. 27323-41-7.

18-FEB-2000. Unger FAbrikker A/S Fredrikstad.
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)
Results: 96-hr algae EC50 = 70 mg/L
Method: Estimated by Calculation
GLP: Not applicable
Test Substance: **27323-41-7.** dodecyl benzenesulphonic acid, compound with 2,2',2"-nitrilotriethanol (1:1)
Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference: **90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 26264-06-2
(a)
Results: 96-hr algae EC50 = 70 mg/L
Method: Estimated by Calculation
GLP: Not applicable
Test Substance: **26264-06-2.** benzenesulphonic acid, dodecyl, calcium salt
Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference: **90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68411-32-5
(a)
Results: 96-hr algae EC50 = 69 mg/L
Method: Estimated by Calculation
GLP: Not applicable
Test Substance: **68411-32-5.** benzenesulphonic acid, dodecyl, branched
Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C11.9
Reference: **90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68953-96-8
(a)
Results: 96-hr algae EC50 = 55 mg/L
Method: Estimated by Calculation
GLP: Not applicable

Test Substance:	**68953-96-8.** benzenesulphonic acid, mono-C11-13-branched alkyl derives., calcium salts
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C13.5
Reference:	**90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68608-88-8

(a)

Results:	96-hr algae EC50 = 68 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68608-88-8.** benzenesulphonic acid, mono-C11-13-branched alkyl derives.
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C11.8
Reference:	**90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 90218-35-2

(a)

Results:	96-hr algae EC50 = 68 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**90218-35-2.** benzenesulphonic acid, dodecyl-, branched, compds with 2-propanamine
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C11.8
Reference:	**90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68608-89-9

(a)

Results:	96-hr algae EC50 = 55 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68608-89-9.** benzenesulphonic acid, mono-C11-13-branched alkyl derives., sodium salts
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C13.5
Reference:	**90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 42615-29-2

(a)

Results:	96-hr algae EC50 = 70 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**42615-29-2.** benzenesulphonic acid, linear alkyl
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference:	**90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68584-26-9

(a)

Results:	96-hr algae EC50 = 60 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**68584-26-9.** benzenesulphonic acid, C10-16-alkyl derives., magnesium salt
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C13
Reference:	**90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 70528-83-5

(a)

Results:	96-hr algae EC50 = 65 mg/L
Method:	Estimated by Calculation
GLP:	Not applicable
Test Substance:	**70528-83-5.** benzenesulphonic acid, dodecyl-, branched, calcium salts
Remarks:	ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12.5
Reference:	**90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability:	2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS No. 68411-30-3

(a)

Species:	*Selenastrum capricornutum* and *Scenedesmus subspicatus*
Endpoint:	Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Results:	E_rC_{50} values ranged from 29 to 35.5 for *S. capricornutum* (two records) E_rC_{50} values ranged from 82 to 163 mg/L for *S. subspicatus* (three records)

Test Substance: C_{10-13} LAS (CAS #**68411-30-3**)

Remarks: A total of 13 algae studies originally were reviewed by HERA in 2004. Eight of these studies were rejected because the test material was not commercial LAS, the study deviated significantly from standard protocols, or non-standard endpoints were measured. The remaining five studies were evaluated for reliability and the results reflect the range of acute E_rC_{50} values obtained for the two most commonly tested algal species. These studies are tabulated and discussed further in the SIAR and SIAP in a weight-of-evidence approach.

Reference: **42.** HERA. 2004. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. **68411-30-3**, Version 2.0 June 2004. http://www.heraproject.com/riskassessment.cfm. .

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Species: *Scenedesmus subspicatus* (Algae)

Endpoint: Biomass **[X]**; Growth rate **[X]**; Other **[ ]**

Exposure period: 72 hour

Results: E_rC_{50} (growth rate) = 127.9 mg/L; E_bC_{50} (biomass) = 43.2 mg/L
NOEC (growth rate) = 2.4 mg/L; NOEC (biomass) = 2.2 mg/L
LOEC (growth rate) = 10 mg/L

Inhibition of cell growth by concentration and duration is shown in the table below:

Cell number (x 10^4 cells/mL)				
	Time Period (hours)			
Test concentration (mg/L)	**0**	**24**	**48**	**72**
Control	2	8	29	95
0.6	2	8	30	89
2.4	2	9	28	85
10	2	9	27	75
40	2	8	20	48
160	2	7	9	8

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: open-system **[X]**; closed-system **[ ]**
Algal growth inhibition test (88/302/EWG) 1988.
Nominal test concentrations were control, 0.6, 2.4, 10, 40, and 160 mg/L. Algae were exposed to LAS in Erlenmeyer flasks in an environmental chamber on a light table at 8000 lux. Cell numbers

were photometrically determined (8 subsets were taken for each concentration).

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: Marlon A 390 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = 11.6; 91.3% activity

Remarks: Initial cell concentrations were 20,000 cells/mL. Cell concentrations at 72 h were 95, 89, 85, 75, 48 and 8 (all x 10^4/mL) for the control, 0.6, 2.4, 10, 40 and 160 mg/L LAS concentrations, respectively. The pH ranged from 7.7 to 7.9 at the beginning of the study and 7.9 to 9.0 at the end of the study. Test temperature was maintained at 24 ± 2 °C. This is a key study for aquatic toxicity to algae (see SIAR Table 12).

Reference: **56.** Scholz, N. 1992. Bestimmung der Auswirkungen von Marlon A 390 auf das Wachstum von *Scenedesmus subspicatus* 86.81. SAG (Algenwachstumshemmtest nach Richtlinie 88/302/EWG) Huels Final Report No. AW-291.

Reliability: 1 Valid without restriction

(c)

Species: *Scenedesmus subspicatus* (Algae)

Endpoint: Biomass **[X]**; Growth rate **[X]**; Other **[ ]**

Exposure period: 72 hour

Results: E_rC_{50} (growth rate) = 82 mg/L; E_bC_{50} (biomass) = 20 mg/L
NOEC (growth rate) = 0.4 mg/L; NOEC (biomass) = 0.1 mg/L

Inhibition of cell growth by concentration and duration is shown in the table below:

Cell number (x 10^4 cells/mL)				
	Time Period (hours)			
Test concentration (mg/L)	**0**	**24**	**48**	**72**
Control	2	9	32	94
0.1	2	9	32	91
0.4	2	9	29	88
1.6	2	9	28	76
6.4	2	9	24	60
25	2	9	21	54
160	2	6	7	7

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: open-system **[X]**; closed-system **[ ]**
Algal growth inhibition test (92/69/EWG)
Nominal test concentrations were control, 0.1, 0.4, 1.6, 6.4, 25 and 160 mg/L. Test concentrations were measured at 0 and 72 h and found to confirm the nominal concentrations. Algae were exposed

to LAS in Erlenmeyer flasks in an environmental chamber on a light table at 8000 lux. Cell numbers were photometrically determined (8 subsets were taken for each concentration).

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = 11.6; 52.1% activity

Remarks: Initial cell concentrations were 20,000 cells/mL. Cell concentrations at 72 h 94, 91, 88, 76, 60, 54 and 7 (all x 10^4/mL) for the control, 0.1, 0.4, 1.6, 6.4, 25 and 160 mg/L LAS concentrations, respectively. The pH ranged from 8.2 to 8.3 at the beginning of the study and 8.0 to 9.4 at the end of the study. Test temperature was maintained at 24 ± 2 °C. This is a key study for aquatic toxicity to algae (see SIAR Table 12).

Reference: **57.** Scholz, N. 1994. Bestimmung der Auswirkungen von Marlon A 350 auf das Wachstum von *Scenedesmus subspicatus* 86.81. SAG (Algenwachstumshemmtest nach Richtlinie 92/69/EWG) Huels Final Report No. AW-372.

Reliability: 1 Valid without restriction

(d)

Species: *Scenedesmus subspicatus* (Algae)

Endpoint: Biomass **[X]**; Growth rate **[ ]**; Other **[ ]**

Exposure period: 96 hour

Results: EC_{50} = 5 mg/L

Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**

Method: DIN 38412 Part 9

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = 11.6

Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Data refer to 100% active ingredient. Test method conforms with OECD-Guideline 201.

Reference: **47.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(e)

Species: *Scenedesmus subspicatus* (Algae)

Endpoint: Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**

Exposure period: 96 hour

Results: EC_{50} = 9 mg/L

Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**

Method: Directive 87/302/EEC, part C, p. 89 "Algal inhibition test"
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-13} LAS, sodium salt; average chain length 11.6 (CAS #**68411-30-3)**
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good.
Reference: **43.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Huels AG, 1/90, N. Scholz, unpublished.
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(f)
Species: *Scenedesmus subspicatus* (Algae)
Endpoint: Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Exposure period: 96 hour
Results: EC_{50} = 30 mg/L
Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: ISO 8692 "Water quality - Fresh water algal growth inhibition test with *Scenedesmus subspicatus* and *Selenastrum capricornutum*"
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{11-13} LAS
Remarks: Information as cited in IUCLID Data Sheet for CAS #**68411-30-3.** Huels AG judged study quality to be good. Nominal concentrations (deviation <3%); BBM medium; pH 6.4-6.7; 20-22ºC. Note that although this was cited in IUCLID as a Procter & Gamble report, Procter & Gamble indicates that it is unlikely that it is one of their reports.
Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, AL/12.
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(g)
Species: *Selenastrum capricornutum* (Algae)
Endpoint: Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Exposure period: 72 hour
Results: EC_{50} = 11 mg/L
Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: ISO 8692 "Water quality - Fresh water algal growth inhibition test with *Scenedesmus subspicatus* and *Selenastrum capricornutum*"
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{11-13} LAS (CAS #68411-30-3)

Remarks: Information as cited in IUCLID Data Sheet for CAS #**68411-30-3.** Huels AG judged study quality to be good. Nominal concentrations (deviation <13%); BBM medium; pH 6.5-6.6; static. Note that although this was cited in IUCLID as a Procter & Gamble report, Procter & Gamble indicates that it is unlikely that it is one of their reports.

Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, AL/10.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(h)

Species: *Selenastrum capricornutum* (Algae)

Endpoint: Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**

Exposure period: 96 hour

Results: EC_{50} = 12.2 mg/L

Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**

Method: EPA, l987.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: C_{10-13} LAS, average chain length 12.3 (CAS #68411-30-3)

Remarks: Information as cited in IUCLID Data Sheet for CAS #**68411-30-3.** Huels AG judged study quality to be good. AAP medium; 24^{+}/-2ºC.

Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, P2636.01.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(i)

Type of Test: Static [X]; semi-static [ ]; flow-through [ ]
Open-system [ ]; closed-system [ ]; not stated [X]

Species: *Chlorella kessleri* (algae)

Exposure Period: 15 days

Effect Criteria: Growth rate

Results: NOEC = 3.1 mg/L
LOEC = 10 mg/L

Analytic Monitoring: Yes [ ]; No [X]; ? [ ]

Method: EPA-600/9-78-018. Algal Assay Bottle Test. Determination of The Inhibitory effect of water constituents on green algae, by William E. Joseph C. Greene, and Tamotsu Shiroyama, Corvallis Environmental Research Laboratory, Corvallis, Oregon.

GLP: Yes [ ]; No [X]; ? [ ]

Test Substance: Marlon A 350, Benzenesulfonic acid, C10-13-alkyl derives., sodium salts (CAS #**68411-30-3.)**; 25.7% activity.

Remarks: No morphological changes were observed. The growth rate was reduced at LAS concentrations of 20 mg/L. Protein analysis indicated that higher concentrations did affect protein synthesis. The NOEC normalized by van de Plassche et al. (1999) to $C_{11.6}$ LAS was 3.5 mg/L.

Reference: **58.** Henkel KGaA, Biological Research and Product Safety/Ecology, unpublished results of study conducted in 1984; test substance Fi 5829.

Reliability: 2 Valid with restrictions. Non-standard length of study; No EC_{50}

(j)

Results: 96-hr algae EC50 = 70 mg/L

Method: Estimated by Calculation

GLP: Not applicable

Test Substance: **68411-30-3.** benzenesulphonic acid, C10-13 alkyl derives., sodium salt

Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12

Reference: **90.** USEPA. OPPT SAR for Anionic Surfactants table

Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

CAS RN 27176-87-0

(a)

Species: *Selenastrum capricornutum* (Algae)

Endpoint: Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**

Exposure period: 96 hour

Results: EC_{50} = 29 mg/L

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: EPA method

GLP: Yes **[ ]** No **[X]** ? **[]**

Test substance: benzene sulfonic acid, dodecyl- (CAS # **27176-87-0**)

Remarks: 1985

Reference: **79.** European Commission. 1992. IUCLID dataset for benzene sulfonic acid, dodecyl- **CAS #27176-87-0**. 1995. cited Galassi et al. 1992. Water Research 26:19-27.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Results: 96-hr algae EC50 = 70 mg/L

Method: Estimated by Calculation

GLP: Not applicable

Test Substance: **27176-87-0.** benzenesulfonic acid, dodecyl
Remarks: ECOSAR Class - Anionic surfactant – alkyl benzene sulfonates; effective alkyl chainlength = C12
Reference: **90.** USEPA. OPPT SAR for Anionic Surfactants table
Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

8.3.4 Toxicity to Bacteria

CAS No. 68411-30-3

(a)
Type: Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: activated sludge
Exposure Period: 15 minute
Results: EC_{50} = 107-152 mg/L
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: ESD-VIII-D-1, Issue II (9/8/80)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-13} LAS (CAS #**68411-30-3**)
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Effect: inhibition of respiration. Nominal concentrations (expected deviation <20%). Mixed Liquor Suspended Solids 53.6-76.1 mg/g VSS/Sewage. Static, 25ºC. Activated sludge (2600 mg SS/L)
Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 27896, 27897, 27915.
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)
Type: Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: *Pseudomonas putida* (Bacteria)
Exposure Period: 18 hour
Results: EC_{50} = 60.9-63.5 mg/L
EC_{10} = 52.7-56.6 mg/L
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: Bacterial toxicity test according to DIN 38412 part 8. A total of 6 concentrations were tested (40-80 mg/L) under GLP conditions.
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Marlon A 390 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = 11.6; activity 91.3%,
Remarks: Results show EC_{50} and EC_{10} values for two tests.

Reference: **85.** Scholz, N. 1993. Bestimmung der bacterientoxizitat von Marlon A 390 in Pseudomonas-zellvermehrungs-Hemmtest. Huels-Final Report No. PZ-93/10.
Reliability: 2 Valid with restrictions

(c)
Type: Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: *Pseudomonas putida* (Bacteria)
Exposure Period: 30 minute
Results: EC_{50} = 350 mg/L
EC_0 = 250 mg/L
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**
Method: DIN 38412 Teil 27 (respiration inhibition test)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Data refer to 100% active ingredient.
Reference: **47.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(d)
Type: Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: *Pseudomonas putida* (Bacteria)
Exposure Period: 16 hour
Results: EC_{50} = 150 mg/L
EC_0 = 50 mg/L
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**
Method: DIN 38412 Teil 8 (cell multiplication inhibition test)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Data refer to 100% active ingredient
Reference: **47.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(e)

Type:	Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species:	*Pseudomonas putida* (Bacteria)
Exposure Period:	30 minute
Results:	NOEC = 64 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	DIN 38412, Teil 27
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	$C_{10\text{-}13}$ LAS, average chain length 11.8 (CAS #**68411-30-3**)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Synthetic water; static; pH 7.2^{+}/-0.2; 20ºC. Effect: Inhibition of oxygen consumption.
Reference:	**47.** European Commission. 2000. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KgaA.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.3.5 Chronic Toxicity to Aquatic Organisms

8.3.5.1 Chronic Toxicity to Fish

CAS No. 68411-30-3

(a)

Type of Test:	Static [ ]; semi-static [X]; flow-through [ ] Open-system [X]; closed-system [ ]; not stated [ ]
Species:	*Brachydanio rerio* (Zebra Fish, fresh water)
Exposure Period:	14 days
Effect Criteria:	Mortality, behavior
Results:	NOEC = 2.0 mg/L LOEC = 4.0 mg/L
Analytic Monitoring:	Yes [ ]; No [X]; ? [ ]
Method:	Based on UBA-Verfahrensvorschlag:Verlaengerter Toxizitaetstest beim Zebrabaerbling *Brachydanio rerio*, Bestimmung der Schwellenkonzentration der letalen und anderer Wirkungen, NOEC, mindestnes 14 Tage. This method conforms with OECD Guideline 204. Ten fish were exposed to each of seven concentrations (0.2, 0.4, 0.8, 1.6, 2.0, 4.0 and 8.0 mg/L) and the controls. Test chambers were 10-L basins containing 5-L of copper- and chlorine-free drinking water, maintained in a 16:8 light:dark illumination cycle. The NOEC normalized by van de Plassche et al. (1999) to $C_{11.6}$ LAS was 2.3 mg/L.
GLP:	Yes [ ]; No [X]; ? [ ]
Test Substance:	Marlon A 350 LAS (CAS #**68411-30-3**; Benzenesulfonic acid, $C_{10\text{-}13}$- alkyl derives., sodium salts, 25.7% activity)

Reference: **86.** Henkel KGaA, Biological Research and Product Safety/Ecology: unpublished results (Test substance number Fi 5959).

Reliability: 2 Valid with restrictions. Duration of test considered too short for a chronic study.

(b)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**

Species: *Pimephales promelas* (Fish, fresh water)

Exposure period: 30 day

Effect criteria: Fry survival

Results: NOEC = 1 mg/L
LOEC = 2 mg/L

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]** HPLC

Methods: Two replicates of 100 egg-fry stage fathead minnows were exposed for 30 days to LAS under the following conditions: Hardness 41 mg/L as $CaCO_3$; pH 7.2; temperature 24^{o}C. The exchange rate was 1 to 3 volume changes/day. Test chambers were 3500 mL volume. The studies were conducted at EG&G Bionomics (now Springborn Smithers Laboratory).

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: Commercial $C_{10\text{-}13}$ LAS, sodium salt (CAS #**68411-30-3**); C_{10} 5%, C_{11} 27%, C_{12} 53%, C_{13} 13%; 2-phenyl 23%.

Remarks: Carboxylated intermediates formed in the biodegradation of LAS exhibit toxicity several orders of magnitude less than LAS; LC_{50} values were >144 mg/L and >52 mg/L for sulfophenyl butarate and sulfophenyl undecanoate, respectively. NOEC based on fry survival. Egg hatchability and fry growth were less sensitive. This is a key study for chronic aquatic toxicity to fish (see SIAR Table 12).

Reference: **54.** Swisher, R.D., Gledhill, W.E., Kimerle R.A. and Taulli, T.A. 1978. Carboxylated intermediates in the biodegradation of linear alkylbenzene sulfonates (LAS). VII International Congress on Surface Active Substance, Proceedings, Moscow, 1976 4:218-230.

Reliability: 2 Valid with restrictions

(c)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**

Species: *Salmo gairdneri* (*Oncorhyncus mykiss*, fish, estuary, fresh water)

Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[X]** Growth

Exposure period: 28 day

Results: NOEC = 0.43-0.89 mg/L

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: Crossland, N O.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{10-13} LAS (CAS #**68411-30-3**)
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Mean NOEC: 0.62 mg/1 (2 tests). Huels AG judged study quality to be good. Tap water with hardness 84-153 mg/L $CaCO_3$; pH 7.1-8.7; flow-through; 14-16ºC; age of fish at start of study: 6 months.
Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, CT/R153/01, CT/R153/06.
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(d)
Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species: *Salmo gairdneri* (Fish, estuary, fresh water)
Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[X]** Growth, Hatching, Survival
Exposure period: 70 day
Results: NOEC = 0.23 mg/L
Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: Unilever Research Protocol, Early Life Stage (ELS) test.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{10-13} LAS (CAS #**68411-30-3**)
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Tap water with hardness 70-133 mg/L $CaCO_3$; pH 7.3-7.8; flow-through; 8.5-11.5ºC; life-stage: ELS.
Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, CT/R118/03.
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(e)
Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species: *Salmo gairdneri* (Fish, estuary, fresh water)
Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[X]** Growth, Hatching, Survival
Exposure period: 70 day.
Results: NOEC = 0.3-0.35 mg/L
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: Unilever Research Protocol.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{10-13} LAS (CAS #68411-30-3)
Remarks: Information as cited in IUCLID Data Sheet for CAS #**68411-30-3.** Mean NOEC: 0.32 mg/1 (2 tests). Huels AG judged study quality to be good. Nominal concentrations (expected <20%). Tap water with hardness 64-159 mg/L $CaCO_3$; pH 6.6-8.0; flow-through; 7.5-15 ºC; life-stage: ELS
Reference: **52.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, CT/R89/01, CT/R89/02.
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(f)
Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**
Species: *Pimephales promelas* (Fish, fresh water)
Exposure period: 28 day
Results: NOEC ($C_{11.8}$) = 0.9 mg/L
NOEC (C_{13}) = 0.15 mg/L
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{10-13} LAS (CAS #**68411-30-3**), average chain lengths 11.8 & 13
Remarks: Observations were made of the number of spawnings, total eggs produced, and number of eggs per female. Data were obtained from the literature.
Reference: **87.** Maki, A.W. 1979. Correlations between *Daphnia magna* and fathead minnow (*Pimephales promelas*), chronic toxicity values for several classes of test substances. J. Fish. Res. Bd Can. 36, 411-421.
Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.3.5.2 Chronic Toxicity to Aquatic Invertebrates (Water-only Exposures)

CAS No. 68411-30-3
(a)
Type of test: static **[ ]**; semi-static **[X]**; flow-through **[ ];** open-system **[ ]**; closed-system **[ ]**
Species: *Daphnia magna* (Crustacea)
Endpoint: Mortality **[X]**; Reproduction rate **[X]**
Exposure period: 21days

Results: NOEC = 1.25-3.25 mg/L; LOEC = 2.25-3.75 mg/L
Geometric Mean NOEC = 1.99 mg/L (mean of studies using 5 different diets)
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**
Method: ASTM proposed standard practice for conducting renewal life cycle toxicity tests with *Daphnia magna*. Draft No. 1, August 1982. Ten 250 m/L beakers were used for each test concentration. Seven beakers contained one daphnid each and three beakers contained five daphnids each, for a total of 22 daphnids per concentration. All conditions were maintained as per protocol.
GLP: Yes **[ ]** No **[]** ? **[X]**
Test substance: Commercial $C_{10\text{-}13}$ LAS, average chain length $C_{11.8}$ (CAS #**68411-30-3**).
Remarks: NOEC and LOEC values represent the range of results from five tests using different diets. Diet had at most a three-fold effect on the results, which is within the variation expected within the tests themselves. Therefore, results of different diets can be considered roughly equivalent to five replications of the same diet. This is a key study for chronic aquatic toxicity to invertebrates (see SIAR Table 12).
Reference: **88.** Taylor, M.J. 1985. Effect of diet on the sensitivity of *Daphnia magna* to linear alkylbenzene sulfonate. In: Cardwell, R.D., Purdy, R. and Bahner, R.C. Aquatic Toxicology and Hazard Assessment. Seventh Symposium pp. 53-72. ASTM STP 854,
American Society for Testing and Materials, Philadelphia.
Reliability: 2. Valid with restrictions

(b)
Type of test: static **[ ]**; semi-static **[** X **]**; flow-through **[ ]**; open-system **[X]**; closed-system **[ ]**
Species: *Daphnia magna* (Crustacea)
Endpoint: Mortality **[ ]**; Reproduction rate **[X]**; Other **[ ]**
Exposure period: 21 day
Results: NOEC = 0.3 mg/L
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: OECD Guide-line 202, part 2 "*Daphnia* sp., Reproduction Test
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: $C_{10\text{-}13}$ LAS, with average chain length of $C_{11.8}$ (CAS #**68411-30-3**)
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Natural water 3x weekly renewal pH 6.0-8.5; 20^{+}/-2 ºC; life-stage: 6-24 h.
Reference: **47.** European Commission. 2000. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.3.6 Toxicity to Terrestrial Organisms

8.3.6.1 Toxicity to Soil Dwelling Organisms

CAS No. 68411-30-3

(a)

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[X] Natural soil**

Species: *Folsomia fimetaria* (Collembola; springtails)

Endpoint: Mortality**[X]**; Weight **[X]**; Other **[X] molting rate, reproduction**

Exposure period: 21 days

Results: Results are shown in the following table. All results are in mg/kg dry weight of soil.

Endpoint	NOEC	LOEC	LC_{10} or EC_{10}	LC_{50} or EC_{50}
Adult survival	>1000	>1000	>1000	>1000
Juvenile survival	500	700	196	570
Reproductive output	500	1000	147	737
Juvenile growth	<200	200	163	896
Molting frequency	<300	300	185	923

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were control, 100, 150, 300, 500, 700 and 1000 mg/kg dry weight. Concentrations for survival and groGrowth of juveniles were control, 200, 3000, 500, 700, and 1000 mg/kg dry weight. Concentrations for molting of juveniles were control, 300 and 600 mg/kg dry weight. In all cases, four replicates per concentration were used. For measurement of molting frequency, juveniles were held singly on a compressed surface of soil in multidishes with 24 circular holes. The multidishes were assessed every second day and exuviae were recorded and removed for a period of 20 days. Deviations from the subsequently developed ISO 11267 protocol included use of adults, use of 20 individuals instead of 10 per test chamber, and an exposure of 21 days instead of 28 days.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Marlon A350 (CAS #**68411-30-3**) $C_{10\text{-}13}$ LAS; 50% active substance; mean chain length of $C_{11.53}$; mean molecular weight 344

Remarks: The most sensitive endpoint was reproduction (EC_{10} = 147 mg/kg dry weight). Nominal concentrations are derived from tables and figures since values were not listed directly in the text. While there were some deviations from the subsequently developed ISO 11267 protocol, the procedures are considered reliable.

Reference: **59.** Holmstrup, M. and Krogh, P.H. 1996. Effects of an anionic surfactant, linear alkylbenzene sulfonate, on survival, reproduction and growth of the soil-living collembolan, *Folsomia fimetaria*. Environ. Toxicol. Chem. 15:1745-1748.

Reliability: 2 Valid with restrictions. Well documented publication, non GLP, EC_x calculation not fully detailed.

CAS No. 42615-29-2

(a)

Title Terrestrial safety assessment of linear alkylbenzene sulfonate

Date of report 1990.

GLP No.

Reference **16. Mieure J., Waters J., Holt M., Matthijs E.** 1990. Terrestrial safety assessment of linear alkylbenzene sulfonate. Chemosphere 21 (1-2): 251-262.

Test substance Benzenesulphonic acid, linear $alkyl_{10\text{-}13,\ mean\ 11.6}$.

Test method OECD 207 (1984).

Stat. method Not indicated.

Test system

Species Earthworm (*Eisenia foetida*), mean weight 660 mg

No. of worms 10 worms/jar, 4 jars/treatment.

Procedure The test was performed at 20±2°C under continuous illumination in 0.9 L glass jars, containing 900 g of wet artificial soil (peat/clay/sand: 10/20/70%). An aqueous solution of LAS was added to the soil. The treatment rates were 63, 125, 250, 500, and 1000 mg/kg soil. Untreated controls were included. Moisture level was maintained at 35±1%.

Observations Mortality, symptoms, body weight on day 7 and 14.

Analysis At 250 mg/kg by HPLC.

Results Reductions in body weights of respectively 14, 33 and 23% were observed at 0, 100 and 500 mg/kg.

Measured concentration was 94% of nominal.

Parameter	**Time [d]**	**Nominal concentration [mg/kg soil]**					
		0	**63**	**125**	**250**	**500**	**1000**
Mortality [%]	14	0	0	0	0	0	5

Conclusions 14-day LC_{50} >1000 mg/kg

Rev. note 1. No positive control included.

Reliability 2 Valid with restrictions. No positive control; non-GLP study

8.3.7 Toxicity to Terrestrial Plants

CAS No. 42615-29-2

(a)

Title	Terrestrial safety assessment of linear alkylbenzene sulfonate	
Date of report	1990.	
GLP	No.	
Reference	**16. Mieure J., Waters J., Holt M., Matthijs E.** 1990. Terrestrial safety assessment of linear alkylbenzene sulfonate. Chemosphere 21 (1-2): 251-262.	
Test substance	Benzenesulphonic acid, linear alkyl, LAS $C_{10\text{-}13,\ mean\ 11.6}$.	
Test method	OECD 208 (1984).	
Stat. method	Not indicated.	
Test system	**Species**	Sorghum (*Sorghum bicolor*) Sunflower (*Helianthus annuus*) Mung bean (*Phaseolus aureus*)
	No. of seeds	8 seeds/pot, 4 pots/treatment.
	Procedure	The test was performed in a greenhouse at 20°C with 14 h light in non-porous plastic plant pots (∅ 10 cm) containing 600 g soil (mixture of grit, loam and fertilizer). A premix was prepared from silver sand and a solution of LAS in water. The premix was blended with the soil (1:9). The treatment rates were 1, 10, 100 and 1000 mg a.i./kg dry soil. Untreated controls were included for sorghum.
	Observations	Emergence on day 7. Growth on day 21.

Conclusion	Sorghum: Emergence [%] was 64-78% for 0-1000 mg/kg; 21-d $EC_{50,growth}$ 167 mg/kg. Sunflower: Emergence [%] was >91% for 1-1000 mg/kg soil; 21-d $EC_{50,growth}$ 289 mg/kg. Mung bean: Emergence [%] was ≥75% for 1-1000 mg/kg soil; 21-d $EC_{50,growth}$ 316 mg/kg. 21-d $NOEC_{growth}$ 100 mg/kg for all species
Rev. note	The information was essentially confined to what is included in the above summary. On the basis of the limited information provided, checking of compliance with guideline requirements was only possible to a limited extent. The determination of the effect concentrations (NOEC and EC50) for growth cannot be checked by individual data.
Reliability	2 Valid with restrictions. Incomplete description.

CAS No. 68411-30-3

(a)

Species:	radish, tomato, oats
Endpoint:	Emergence **[ ]**; Growth **[X]**; Other **[ ]**
Exposure period:	14 day
Results:	EC_{50} >77.1 mg/kg soil dw NOEC = 25.7 mg/kg soil dw
Method:	OECD Guide-line 208 "Terrestrial Plants, Growth Test".
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	Commercial LAS with an average carbon chain length of $C_{11.8}$.
Remarks:	Information as cited in IUCLID Data Sheet for CAS #**68411-30-3.** The substance was tested in the range of 2.57 to 257 mg MBAS/kg Nominal concentrations, synthetic soil, static, pH 5.0-7.5, temperature 20-25 ºC. Results are expressed as mg MBAS per kg soil. First Observed Effect Concentration (FOEC) is 77.1 mg MBAS/kg, EC50 is about 77.1 but below 257 mg MBAS/kg.
Reference:	**47.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished data (Registry No. 5929).
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Species:	*Brassica rapa* (Dicotyledon)
Endpoint:	Emergence **[ ]**; Growth **[ ]**; Other **[X]** emergence of seedlings
Exposure period:	21 day
Results:	NOEC = 50 mg/kg soil dw FOEC = 150 mg/kg soil dw
Method:	EEC Directive 79/831, Annex V; EEC Ring Test C (L1) 3: Higher Plant, 1986.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks:	Data refer to 100% active ingredient
Reference:	**47.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(c)

Species:	*Lycopersicum esculentum* (tomato)
Endpoint:	Emergence **[ ]**; Growth **[ ]**; Other **[X]** emergence of seedlings
Exposure period:	21 day

Results:	NOEC = 50 mg/kg soil dw FOEC = 150 mg/kg soil dw
Method:	EEC Directive 79/831, Annex V; EEC Ring Test C (L1) 3: Higher Plant, 1986.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks:	Data refer to 100% active ingredient
Reference:	**47.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(d)

Species:	*Avena sativa* (Monocotyledon)
Endpoint:	Emergence **[ ]**; Growth **[ ]**; Other **[X]** emergence of seedlings
Exposure period:	21 day
Results:	NOEC = 50 mg/kg soil dw FOEC = 150 mg/kg soil dw
Method:	EEC Directive 79/831, Annex V; EEC Ring Test C (L1) 3: Higher Plant, 1986.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks:	Data refer to 100% active ingredient
Reference:	**47.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.4 Human Health Toxicology Endpoints

8.4.1 Acute Toxicity

8.4.1.1 Acute Oral Toxicity

CAS No. 26264-05-1

(a)

Title	Defined oral LD_{50}
Date of report	October 8, 1980.
GLP	No data
Reference	**32. Wo C., Shapiro R**., 1980. Report T-1137. Product Safety Labs

Test substance	Benzenesulfonic acid, dodecyl-, compd. With isopropylamine (1:1), purity 90.9%.	
Guideline	Defined oral LD50. Adapted from appraisal of the Safety of Chemicals in Foods, Drugs and Cosmetics, by the Association of Food and Drug Officials of the United States, 1965.	
Stat. method	Litchfield-Wilcoxin (Probit analysis).	
Test system	**Species**	Rat (Sprague-Dawley), weight 200-300 g.
	No. of animals	5/sex/dose group.
	Dosage	Single dose by oral gavage of 1.0, 1.5, 2.0, 2.5 and 3.0 mL/kg bw.
	Observations	Mortality/clinical signs daily for 14 days. Body weight on day 0 and 14. Macroscopy on animals that died.

Results

Dose [mL kg bw] \ effect		**1.0**		**1.5**		**2.0**		**2.5**		**3.0**		**DR**	
Sex	**Day**	**M**	**F**	**M**	**F**	**M**	**F**	**M**	**F**	**M**	**F**	**M**	**F**
Mortality	0-14	1/5		4/5		4/5		3/5	5/5	5/5	5/5	x	x
Body weight gain survivors	0-14	No treatment related effects							N/A	N/A	N/A		
Clinical signs	0-14	No treatment related effects											
Necropsy(A)				+		+		+	+	+	+		

(A) Pulmonary haemorrhage among animals that died.

Oral LD_{50} 1.8 ml/kg bw which is equivalent to 1300 mg/kg bw

Conclusions

Reliability 2 Valid with restrictions. Only partial report available.

CAS No. 26264-05-1

(b)

Species:	rat
Results:	LD50 = 1836 mg/kg bw
Test Substance:	Benzenesulfonic acid, dodecyl-, compd with isopropylamine (1:1), purity 90%
Remarks:	test guideline not specified
Reference:	**22.** Rhodia MSDS RHODOCAL®330. 1998.
Reliability:	4 Not assignable. Secondary literature.

CAS No. 27323-41-7

(a)

Species:	not indicated
Results:	LD50 = 2320 mg/kg bw
Test Substance:	CAS #**27323-41-7**

Remarks:	none
Reference:	**37.** European Commission. 2000. IUCLID Dataset for dodecylbenzenesulphonic acid, compound with 2,2',2"-nitrilotriethanol (1:1); CAS No. 27323-41-7. 18-FEB-2000. Unger Fabrikker A/S Fredrikstad.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Title	Acute oral toxicity studies with ten samples in albino rats	
Date of report	May 29, 1973	
GLP	No	
Reference	**9. Kretchmar B**. 1973. Acute oral toxicity studies with ten samples in albino rats. Industrial Bio-test Laboratories, Inc.	
Test substance	Benzenesulfonic acid, dodecyl-, compd. With 2,2',2''-nitrilotris(ethanol)(1:1), purity 25%.	
Guideline	Not indicated.	
Test system	**Species**	Rat.
	No. of animals	Not indicated.
	Dosage/observations	Not indicated.
Stat. method	Weil, Thompson.	
Results	Limited to LD_{50}-value.	
Conclusions	Oral LD_{50} 1653 (±238) mg a.i./kg bw.	
Rev. note	Only select pages of the report were available.	
Reliability	4 Incomplete report.	

(c)

Title	Final report on the safety assessment of sodium dodecylbenzenesulfonate/TEA-dodecylbenzenesulfonate/sodiumdecylbenzenesulfonate	
Date of report	1997.	
GLP	No data	
Reference	**1. Cosmetic, Toiletry and Fragrance Association (CTFA).** 1997. CTFA Final report on Na/TEA DDBS.	
Test substance	Benzenesulfonic acid, dodecyl-, compd. With 2,2',2"-nitrilotris(ethanol) (1:1).	
Guideline	Not indicated.	
Stat. method	Not applicable.	
Test system	**Species**	Rat (Sprague-Dawley).

	No. of animals	5/sex/dose group.
	Dosage	Single oral administration of 91, 195, 420, 906 and 1953 mg/kg bw (vehicle water, dosing volume 0.464-10 ml/kg).
	Observations	Mortality/clinical signs during 14 days. Necropsy on day 14.
Results	No deaths, diarrhea among animals.	
Conclusions	Oral LD_{50} >10 ml/kg bw ⇔ >1953 mg/kg bw.	
Rev. note	The report was limited to the above mentioned.	
Reliability	2 Valid with Restrictions. A CTFA Cosmetic Ingredient Review	

CAS No.26264-06-2

(a)

Title	MSDS Rhodacal® CA/70
Date of report	August 17, 1999.
GLP	No data
Reference	**21. Rhodia.** 1998. MSDS RHODOCAL®CA/70
Test substance	Benzenesulfonic acid, dodecyl-,calcium salt, purity 69-71%.
Guideline	Not specified.
Toxicity	LD50-rat 1.8 mL/kg ⇔ 1.3 g a.i./kg = 1300 mg/kg bw
Reliability	4 Not Assignable. Secondary literature

CAS No. 68411-32-5

(a)

Title	Akute orale Toxizität von Marlon A 386 für Ratten	
Date of report	February 15, 1984.	
GLP	No data	
Reference	**15. Mürmann P**. 1984. Akute orale Toxizität von Marlon A386. Chemische Werke Hüls	
Test substance	Benzenesulfonic acid, dodecyl-, branched; purity 86%	
Guideline	OECD 401.	
Stat. method	Lichtfield and Wilcoxon.	
Test system	**Species**	Rat (Bor: WISW), mean weight 123-146 g.
	No. of animals	5/sex/dose group.
	Dosage	Single oral administration of 1250, 1415, 1580 and 1990 mg/kg bw (vehicle water, dosing volume 10 ml/kg); no controls; feeding *ad libitum* (food was withheld ~16 h prior to dosing).
	Observations	Mortality/clinical signs several times during the first

6 h and daily until day 14.
Body weights on day 0, 1, 7 and 14.
Necropsy on day 14.

Results

Dose [mg a.i./kg bw] \ effect		**1250**		**1415**		**1580**		**1990**		**DR**	
Sex	**Day**	**M**	**F**	**M**	**F**	**M**	**F**	**M**	**F**	**M**	**F**
Mortality	1-14	0/5	4/5	5/5	3/5	4/5	5/5	5/5	5/5		
Clinical signs(A)	1-14	+	+	+	+	+	+	+	+		
Body weight gain	1-15	No treatment related effects									
Necropsy(B)	15	+		+		+		+			

(A) Clinical observations included piloerection, hunched posture, diarrhoea, difficult respiration, nasal bleedings, uncoordinated movements, ataxia and (minor) sedation during day 1-5.
(B) Findings consisted of redness of the mucous membrane of the stomach and intestine, hyperaemia of the stomach, adhesions in stomach, liver, spleen and kidneys with peritoneum.

Conclusions Oral LD_{50} 1260 mg/kg bw ⇔ 1080 mg a.i./kg bw (95% C.I. 970-1210 mg a.i./kg bw).

Reliability 2 Valid with restrictions. Non-GLP study

CAS No. 68608-88-8

(a)

Title Toxicologic studies with branched and linear alkyl benzene sulfonates in rats

Date of report 1965.

GLP No data

Reference **17. Oser B., Morgareidge K.** 1965. Toxicologic studies with branched and linear alkyl benzene sulfonates in rats. Toxicol. Appl. Pharmacol. 7: 819-825

Test substance Benzenesulfonic acid, mono-C11-13-branched alkyl derivs.) (C_{10}-C_{14}), purity 87.1% (sodium sulfate 10.5%, water 2.2 %, oil 0.9%).

Guideline Hagan (1959).

Stat. method Calculation by method of Miller and Tainter.

Test system

Species Rat (FDRL(Wistar)).

No. of animals 3/sex/dose group.

Procedure Single dose by oral gavage (10% dispersion in water).

Observations Mortality/clinical signs at least daily during 14 days after dosing;
Body weights on day 0, 7 and 14;
Necropsy on day 14 or on day of death.

Conclusions Oral LD_{50} 520 mg a.i./kg bw.

Reliability 2 Valid with restrictions. Published but no lab report

CAS No. 90218-35-2

(a)

Type:	LD_0 [ ]; LD_{100} [ ]; LD_{50} [**X**]; LDL_0 [ ]; Other [ ]
Species/strain:	rat / Sprague Dawley
Value:	1.8 mL/kg bw
Method:	Adapted from Association of Food and Drug Officials of the US, 1965. Five male and five female rats (200–300 grams) were given doses of 1.0, 1.5, 2.0, 2.5 or 3.0 ml/kg by gavage. Animals were observed daily for mortality and other signs of gross toxicity for 14 days after the single dose. Final body weights were recorded and gross necropsies were performed on all mortalities. Temperature was maintained at 68-72^{o}F and photoperiod was a 12 hr light-dark cycle.
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	Siphonate 330; alkyl aryl sulfonate 90.9% active; a clear brown-gold viscous liquid; Lot #B949G9 (CAS #**90218-35-2**; Benzenesulfonic acid, dodecyl-, branched, compds with 2-propanamine)
Remarks:	Combined mortalities (males and females) were 10, 40, 40, 80 and 100% from low to high dose. Females were more sensitive. No control results were reported. Pulmonary hemorrhage was observed in mortalities. The LD50 was calculated by the Litchfield-Wilcoxin method of Probit Analysis.
Reference:	**36.** ALCOLAC, Inc (Rhodia) Product Safety Labs Test report No. T-1137 / PS-1763; Defined Oral LD50; October 8, 1980.
Reliability:	2 Valid with restrictions (No controls results were reported; Test substance [CAS RN] confirmed by sponsor at time of robust summary preparation, but not included in report.)

CAS No. 42615-29-2

(a)

Title	Toxicologic studies with branched and linear alkyl benzene sulfonates in rats
Date of report	1965
GLP	No data
Reference	**17. Oser B., Morgareidge K.** 1965. Toxicologic studies with branched and linear alkyl benzene sulfonates in rats. Toxicol. Appl. Pharmacol. 7: 819-825
Test substance	Benzenesulphonic acid, linear alkyl (C_9-C_{15}), purity 39.5% (sodium sulphate 8.8%, water 50.9 %, free alkali (NaOH) 0.05%, unidentified 0.64%).

Guideline	Hagan (1959)	
Stat. method	Calculation by method of Miller and Tainter.	
Test system	**Species**	Rat (FDRL(Wistar)).
	No. of animals	3/sex/dose group.
	Procedure	Single dose by oral gavage (10% dispersion in water).
	Observation	Mortality/clinical signs at least daily during 14 days after dosing; Body weights on day 0, 7 and 14; Necropsy on day 14 or on day of death.
Conclusions	Oral LD_{50} 650 mg a.i./kg bw.	
Rev. note	1. No individual data were presented. 2. Equivalent doses as 10 and 40% dispersion were given at 600 and 1580 mg/kg. Mortality was not affected by the use of a more concentrated suspension, but a higher incidence of diarrhoea was noted at the most concentrated suspension.	
Reliability	2 Valid with restrictions. Limited report, non-GLP study.	

CAS No. 68411-30-3

(a) **(Rat)**

Type:	LD_0 [ ]; LD_{100} [ ]; LD_{50} [**X**]; LDL_0 [ ]; Other [ ]
Species/strain:	rat
Value:	1080 mg/kg bw
Method:	OECD Guide-line 401 "Acute Oral Toxicity" 1981. Five male and five female rats were given LAS doses of 1075, 1220, 1360, 1710 or a control by gavage. Body weight and other signs were measured on days 7 and 14. Temperature was maintained at 20^{+}/-1^{o}C with a 12 hr light-dark cycle. Animals were observed for 14 days after dosing.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 386 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; Activity: 86%
Remarks:	Symptoms beginning about 30 minutes past application included diarrhea, squatting attitude, breathing difficulties, nose bleeding, ataxia, and lethargy. These symptoms had disappeared in surviving animals by 120 hours. Virtually all animals died in doses of 1220 mg/kg and above. Note that all doses are corrected for 86% activity. The original doses were 1250, 1415, 1580 and 1990 mg/kg.
Reference:	**60.** Murmann, P. 1984a. Akute orale Toxizitat von Marlon A 386 fur Ratten. Huels Report No. 0191.
Reliability:	2 Valid with restrictions

(b)

Type:	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	rat
Value:	1630 mg/kg bw
Method:	OECD Guide-line 401 "Acute Oral Toxicity" 1981. Five male and five female rats were given LAS doses of 1260, 1580, 1785, and 1990 or a control by gavage. Body weight and other signs were measured on days 7 and 14. Temperature was maintained at 20^{+}/-1^{o}C with a 12 hr light-dark cycle. Animals were observed for 14 days after dosing.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; Activity: 50%
Remarks:	Symptoms beginning about 1-4 hours past application included diarrhea, squatting attitude, breathing difficulties, nose bleeding, ataxia, and lethargy. The symptoms in the lower doses disappeared with 24 to 48 hours. Symptoms disappeared in the 1785 mg/kg dose and higher within 8 days. Virtually all animals died in doses of 1785 mg/kg and above. Note that all doses are corrected for 50% activity. The original doses were 2510, 3160, 3570 and 3980 mg/kg.
Reference:	**61.** Murmann, P. 1984b. Akute orale Toxizitat von Marlon A 350 fur Ratten. Huels Report No. 209.
Reliability:	2 Valid with restrictions

(c)

Type:	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	rat
Value:	1410 mg/kg bw
Method:	OECD Guide-line 401 "Acute Oral Toxicity" 1981. Five male and five female rats were given LAS doses of 1190, 1500 and 1890 or a control by gavage. Body weight and other signs were measured on days 7 and 14. Temperature was maintained at 20^{+}/-1^{o}C with a 12 hr light-dark cycle. Animals were observed for 14 d. after dosing.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 330 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; Activity: 30%.
Remarks:	Symptoms beginning about 90 minutes past application included diarrhea, squatting attitude, breathing difficulties, nose bleeding, ataxia, and lethargy. These symptoms had disappeared in surviving animals by 72 hours. Virtually all animals died in doses of 1500 mg/kg and above. Note that all doses are corrected for 30% activity. The original doses were 3980, 5010 and 6310 mg/kg.
Reference:	**62.** Murmann, P. 1984c. Akute orale Toxizitat von Marlon A 330 fur Ratten. Huels Report No. 0186.
Reliability:	2 Valid with restrictions

(d)

Type:	LD_0 [ ]; LD_{100} [ ]; LD_{50} [**X**]; LDL_0 [ ]; Other [ ]
Species/strain:	rat
Value:	LD_{50} for male animals: 1460 mg/kg LD_{50} for female animals: 1470 mg/kg
Method:	Male and female rats were given a single dose of LAS by gavage and observed for mortality.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	$C_{10\text{-}13}$ LAS, sodium salt (CAS #**68411-30-3**) $<C_{10}$ 0.1%, C_{10} 10.1%, C_{11} 33.7%, C_{12} 31%, C_{13} 25.1%.; average alkyl chain length = $C_{11.7}$; activity: 99.5%
Remarks:	Information as reported in IPCS document.
Reference:	**62.** Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M., and Fukushima, A. 1978. Acute, subacute and chronic toxicity of magnesium linear alkylbenzene sulfonate (LAS-Mg). J. Med. Soc. Toho, Japan. 25 (5-6):850-875 (in Japanese). Referenced in IPCS, Environmental Health Criteria 169. Linear Alkylbenzene Sulfonates and Related Compounds, WHO.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(e)

Type:	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	mouse
Value:	LD_{50} male animals: 2160 mg/kg LD_{50} female animals: 2250 mg/kg
Method:	Male and female mice were given a single dose of LAS and observed for mortality.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	$C_{10\text{-}13}$ LAS, sodium salt (CAS #**68411-30-3**). $<C_{10}$ 0.1%, C_{10} 10.1%, C_{11} 33.7 %, C_{12} 31%, C_{13} 25.1%; average alkyl chain length = $C_{11.7}$; activity: 99.5%
Remarks:	Information as cited in IPCS document.
Reference:	**63.** Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M., and Fukushima, A. 1978. Acute, subacute and chronic toxicity of magnesium linear alkylbenzene sulfonate (LAS-Mg). J. Med. Soc. Toho, Japan. 25 (5-6):850-875 (in Japanese). Referenced in IPCS, Environmental Health Criteria 169. Linear Alkylbenzene Sulfonates and Related Compounds, WHO.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.4.1.2 Acute Inhalation Toxicity

CAS No. 25155-30-0 (*from the LAS HPV category that includes supporting chemical CAS No.68411-30-3)*

(a)

Type:	LC_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[]**; LDL_0 **[ ]**; Other **[X]** Approximate lethal concentration (ALC)
Species/strain:	Rat/Male Crl: CD(SD)BR
Exposure:	single 4-hour period
Value:	310 mg/m^3 of particulate
Method:	Groups of six male 8-week old rats were restrained in perforated, stainless steel cylinders with conical nose pieces. Exposure was nose-only to an aerosol atmosphere for 4 hours. After exposure, rats were returned to their cages and observed for clinical signs for 14 days. Mean measured concentrations in the test chambers were 65, 120, 260 and 310 mg/m^3. Chamber temperature ranged between 25-26 degrees.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	.....LAS (CAS #25155-30-0); dodecylbenzene sulfonic acid, sodium salt; activity 98%
Remarks:	The ALC is defined as the lowest atmospheric concentration generated that caused death in one or more rates either on the day of exposure or within 14 days post exposure. No mortality occurred at concentrations up to 260 mg/m^3. At 310 mg/m^3 one rat died during exposure and two rats died one day post exposure. The test material is considered moderately toxic by inhalation. However, it is important to note that this laboratory exposure is not representative of the possible LAS exposure during actual use. In this study, animals were given high exposures to respirable-sized particles (MMAD at 310 mg/m^3 = 2.5 microns). Spray products containing LAS are designed to produce large particle sizes. These large particles are needed for efficient delivery of the spray to the surfaces being cleaned. This results in particle sizes that are much larger than the respirable particle sizes used in testing and therefore would not be able to reach far into the lungs where effects would occur. Given this lack of relevance to real-world exposure potential, this use of this study beyond establishing the relative toxicity of the chemical is limited.
Reference:	**72.** Kinney, L.A. 1985. Approximate lethal concentrations (ALCs) by inhalation of sodium lauryl sulphate and sodium dodecylbenzene sulfonate. Dupont Haskell Laboratory Report No. 474-84.
Reliability:	2 Valid with restrictions.

8.4.1.3 Acute Dermal Toxicity

CAS No. 27323-41-7

(a)

Title	Final report on the safety assessment of sodium dodecylbenzenesulfonate/TEA-dodecylbenzenesulfonate/sodiumdecylbenzenesulfonate	
Date of report	1997	
GLP	No data	
Reference	**1. Cosmetic, Toiletry and Fragrance Association (CTFA).** 1997. CTFA Final report on Na/TEA DDBS.	
Test substance	Benzenesulfonic acid, dodecyl-, compd. with 2,2',2"-nitrilotris(ethanol) (1:1).	
Guideline	Dermal - Not indicated.	
Stat. method	Not applicable.	
Test system	**Species**	Rabbit (New Zealand White).
	No. of animals	8.
	Dosage	Single application of 4199 mg/kg bw (vehicle water) to the clipped skin under occlusion for 24 hours..
	Observations	Mortality/clinical signs during 14 days. Necropsy on day 14.
Results	No deaths, diarrhea and emaciation in two animals, erythema.	
Conclusions	Dermal LD_{50} >21.5 ml/kg bw ⇔ >4199 mg/kg bw.	
Reliability	2 Valid with restrictions. CTFA Cosmetic Ingredient Review	

8.4.1.4 Acute Toxicity, Other Routes of Administration

CAS No. 68411-30-3

(a)

Type:	LD_0 **[ ]**; LD100 **[ ]**; LD50 **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	rat
Administration:	i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[X]**; other **[ ]**
Value:	Females = 810 mg/kg; males = 840 mg/kg bw
Method:	Rats were given subcutaneous injections of LAS
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	..... C_{10-13} LAS, sodium salt (CAS #**68411-30-3**) <C_{10} 0.1%, C_{10} 10.1%, C_{11} 33.7 %, C_{12} 31%, C_{13} 25.1%; average alkyl chain length = $C_{11.7}$; activity: 99.5%
Remarks:	Information as cited in IPCS document.
Reference:	**63.** Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M., and Fukushima, A. 1978. Acute, subacute and chronic toxicity of magnesium linear alkylbenzene sulfonate (LAS-Mg). J. Med. Soc. Toho, Japan. 25

(5-6):850-875 (in Japanese). Referenced in IPCS, Environmental Health Criteria 169. Linear Alkylbenzene Sulfonates and Related Compounds.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**

Species/strain: mouse

Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[X]**; other **[ ]**

Value: Females = 1400 mg/kg; males = 1250 mg/kg bw

Method: Mice were given subcutaneous injections of LAS.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: ..... C_{10-13} LAS, sodium salt (CAS #**68411-30-3**) <C_{10} 0.1%, C_{10} 10.1%, C_{11} 33.7 %, C_{12} 31%, C_{13} 25.1%; average alkyl chain length = $C_{11.7}$; activity: 99.5%

Remarks: Information as cited in IPCS document.

Reference: **63.** Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M., and Fukushima, A. 1978. Acute, subacute and chronic toxicity of magnesium linear alkylbenzene sulfonate (LAS-Mg). J. Med. Soc. Toho, Japan. 25 (5-6):850-875 (in Japanese). Referenced in IPCS, Environmental Health Criteria 169. Linear Alkylbenzene Sulfonates and Related Compounds.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.4.2 Corrosiveness/Irritation

8.4.2.1 Skin Irritation/Corrosion

CAS No. 26264-05-1

(a)

Title	Primary skin irritation
Date of report	September 18, 1980.
GLP	No data
Reference	**31. Wo C., Shapiro R.** 1980. Report T-1047 (E00617-5). Product Safety Labs
Test substance	Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1), purity 90.9%.
Guideline	FHSLA 16 CFR 1500.
Stat. method	Not applicable.

Test system	**Species**	Rabbit (New Zealand White).
	No. of animals	6 (sex not indicated)
	Dosage	Application of 0.5 ml test substance (no vehicle) on ~6.25 cm^2 of the clipped skin (intact and abraded) under semi-occlusion for 24 hours.
	Observations	Skin observations at 24 and 72 h after application.

Results

	Mean score	
Time	**Erythema**	**Oedema**
24 h	1.83	2.33
72 h	3.00	1.67

E=erythema O=oedema

Conclusions Irritating.

Rev. note 1. The application time was 24 h, which is considered to be a worst case situation (OECD 404, 4 h application).

Reliability 2 Valid with restrictions. Only incomplete lab report available

CAS No. 27323-41-7

(a)

Species/strain:	not indicated
Results:	Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**
Test Substance:	CAS #**27323-41-7**
Remarks:	none
Reference:	**37.** European Commission. 2000. IUCLID Dataset for dodecylbenzenesulphonic acid, compound with 2,2',2"-nitrilotriethanol (1:1); CAS No. 27323-41-7. 18-FEB-2000. Unger Fabrikker A/S Fredrikstad.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Title	D.O.T. corrosivity study (Modified)
Date of report	September 13, 1993.
GLP	No (Quality Assurance Statement included).
Reference	**11. Kukulinski M**. 1993. D.O.T. Corrosivity (modified). Tox Monitor Laboratories
Test substance	***Test 1*: Benzenesulfonic acid, dodecyl-, compd. with 2,2',2''-nitrilotris(ethanol)(1:1), purity 60% (40% water),** *Test 2*: Benzenesulfonic acid, dodecyl-, branched) (Benzenesulfonic acid, mono-C11-13-branched alkyl), purity 93-95% (1% sulfuric acid,

0.7% water).

Guideline Not indicated.

Test system Species: Rabbit (New Zealand White), 8-10 weeks old.
No. of animals: 3 (sex not indicated).
Dosage: Application of 0.5 g test substance on the skin under occlusion for 4 hours.
Observations: Skin observations at 4, 24, 48 and 72 h after application.

Stat. Method Not applicable.

Results ***Test 1***

Animal	**1**		**2**		**3**	
Time	**E**	**O**	**E**	**O**	**E**	**O**
4 h	1	1	1	1	1	1
24 h	2	2	1	1	3	2
48 h	3	2	3	2	3	2
72 h	3	2	3	1	3	2

E=erythema O=oedema

Conclusion Irritating

Results ***Test 2***

Animal	**1**		**2**		**3**	
Time	**E**	**O**	**E**	**O**	**E**	**O**
4 h	1	1	1	2	1	1
24 h	2	2	2	2	2	2
48 h	2	1	3	2	3	2
72 h	2	1	2	2	3	2

E=erythema O=oedema

Conclusion Irritating.

Rev. note 1. The test was performed with occlusive dressing. This is considered to represent a worst case situation, since the occlusion is expected to increase penetration through the skin.

Reliability 2 Valid with Restrictions – Note 1

CAS No. 26264-06-2

(a)

Title MSDS Rhodacal® CA/70

Date of report August 17, 1999.

GLP No data

Reference **21. Rhodia.** 1998. MSDS RHODOCAL®CA/70

Test substance Benzenesulfonic acid, dodecyl-,calcium salt, purity 69-71%.

Guideline Not specified.
Skin irritation Moderately irritating in rabbit.
Reliability 4 Not assignable. Secondary literature

CAS No. 68411-32-5
(a)
Title D.O.T. corrosivity study (Modified)
Date of report September 13, 1993.
GLP No (Quality Assurance Statement included).
Reference **11. Kukulinski M**. 1993. D.O.T. Corrosivity (modified). Tox Monitor Laboratories
Test substance *Test 1*: Benzenesulfonic acid, dodecyl-, compd. with 2,2',2''-nitrilotris(ethanol)(1:1), purity 60% (40% water),
***Test 2*: Benzenesulfonic acid, dodecyl-, branched) (Benzenesulfonic acid, mono-C11-13-branched alkyl), purity 93-95% (1% sulfuric acid, 0.7% water).**
Guideline Not indicated.
Test system Species Rabbit (New Zealand White), 8-10 weeks old.
No. of animals 3 (sex not indicated).
Dosage Application of 0.5 g test substance on the skin under occlusion for 4 hours.
Observations Skin observations at 4, 24, 48 and 72 h after application.
Stat. Method Not applicable.
Results ***Test 1***

Animal	**1**		**2**		**3**	
Time	**E**	**O**	**E**	**O**	**E**	**O**
4 h	1	1	1	1	1	1
24 h	2	2	1	1	3	2
48 h	3	2	3	2	3	2
72 h	3	2	3	1	3	2

E=erythema O=oedema
Conclusion Irritating
Results ***Test 2***

Animal	**1**		**2**		**3**	
Time	**E**	**O**	**E**	**O**	**E**	**O**
4 h	1	1	1	2	1	1
24 h	2	2	2	2	2	2
48 h	2	1	3	2	3	2
72 h	2	1	2	2	3	2

E=erythema O=oedema

Conclusion Irritating.
Rev. note 2. The test was performed with occlusive dressing. This is considered to represent a worst case situation, since the occlusion is expected to increase penetration through the skin.
Reliability 2 Valid with Restrictions – Note 1

CAS No. 68608-88-8
(a)
Title D.O.T. corrosivity study (Modified)
Date of report April 21, 1993.
GLP No (Quality Assurance Statement included).
Reference **13. Kukulinski M**. 1993. D.O.T. Corrosivity (modified). Tox Monitor Laboratories
Test substance Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., purity 96% (2% sulfuric acid, 2% benzene (tetrapropenyl derivs).
Guideline Not indicated.
Test system
Species Rabbit (New Zealand White), 8-10 weeks old.
No. of animals 3 (sex not indicated).
Dosage Application of 0.5 g test substance on the skin under occlusion for 4 hours.
Observations Skin observations at 4, 24, 48 and 72 h after application.
Stat. Method Not applicable.

Test 1 *(90% solution in distilled water)*

Results

Animal	**1**		**2**		**3**	
Time	**E**	**O**	**E**	**O**	**E**	**O**
4 h	4	2	4	2	3	2
24 h	4	2	4	1	4	1
48 h	4	1	4	1	4	1
72 h	4	1	4	1	4	1

E=erythema O=oedema
Conclusion Irritating

Results ***Test 2*** *(60% solution in distilled water)*

Animal	**1**		**2**		**3**	
Time	**E**	**O**	**E**	**O**	**E**	**O**
4 h	3	1	4	1	2	1
24 h	4	1	4	1	3	1
48 h	4	1	4	1	3	1
72 h	4	1	4	1	4	1

E=erythema O=oedema
Conclusion Irritating.

Results ***Test 3*** *(30% solution in distilled water)*

Animal	**1**		**2**		**3**	
Time	**E**	**O**	**E**	**O**	**E**	**O**
4 h	1	0	2	1	2	2
24 h	2	1	2	1	2	1
48 h	2	1	2	1	3	1
72 h	3	1	3	1	3	1

E=erythema O=oedema

Conclusion Irritating.

Rev. note 1. The test was performed with occlusive dressing. This is considered to represent a worst case situation, since the occlusion is expected to increase penetration through the skin.

Reliability 2 Valid with restrictions – Note 1

(b)

Title D.O.T. corrosivity study (Modified)

Date of report March 13, 1993.

GLP No

Reference **12. Kukulinski M**. 1993. D.O.T. Corrosivity (modified). Tox Monitor Laboratories

Test substance Benzenesulfonic acid, mono-C11-13-branched alkyl, purity 96% (2% sulfuric acid, 2% benzene (tetrapropenyl derivs.)

Guideline Not indicated.

Test system

Species Rabbit (New Zealand White), 8-10 weeks old.

No. of animals 3 (sex not indicated).

Dosage Application of 0.5 g test substance on the skin under occlusion for 4 hours.

Observations Skin observations at 4, 24, 48 and 72 h after application.

Stat. method Not applicable.

Results

Animal	**1**		**2**		**3**	
Time	**E**	**O**	**E**	**O**	**E**	**O**
4 h	2	2	2	2	1	1
24 h	2	2	3	3	2	2
48 h	2	2	3	3	2	2
72 h	3	3	3	3	3	3

E=erythema O=oedema

Conclusion Irritating.

Rev. note 1. The test was performed with occlusive dressing. This is considered

to represent a worst case situation, since the occlusion is expected to increase penetration through the skin.

Reliability 2 Valid with restrictions – Note 1

CAS No. 90218-35-2

(a)

Species/strain	rabbit / New Zealand Albino
Results:	Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[ ]**; Moderate irritating **[X]**; Slightly irritating **[ ]**; Not irritating **[ ]**
Classification:	Highly corrosive (causes severe burns) **[ ]**; Corrosive (causes burns) **[ ]**; Irritating **[X]**; Not irritating **[ ]**
Method:	Primary Skin Irritation - FHSLA 16 CFR 1500. Six rabbits received 0.5 ml of 90.9% active material to the shaved intact skin. Patches were applied and animals immobilized for 24 hours after which test sites were washed to prevent further exposure. Skin lesions were evaluated and scored at 24 and 72 hours. Temperature was maintained at 68-72^{o}F and photoperiod was a 12 hr light-dark cycle.
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	Siphonate 330; alkyl aryl sulfonate 90.9% active; a clear brown-gold viscous liquid Lot #B949G9 (CAS #**90218-35-2**; Benzenesulfonic acid, dodecyl-, branched, compds with 2-propanamine).
Remarks:	Primary irritation score 4.42. Individual scores: edema: 8.00, erythema: 9.66
Reference:	**35.** ALCOLAC, Inc (Rhodia) Product Safety Labs Test report No. T-1047 / PS-1762; Primary Skin Irritation; September 18, 1980.
Reliability:	2 Valid with restrictions (Test substance [CAS RN] confirmed by sponsor at time of robust summary preparation, but not included in report.)

(b)

Species/strain	rabbit / New Zealand White
Results:	Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ];** Non-corrosive **[X]**
Classification:	Highly corrosive (causes severe burns) **[ ]**; Corrosive (causes burns) **[ ]**; Irritating **[]**; Not irritating **[ ]**; Non-corrosive **[X]**
Method:	Skin Corrosion according to U.S. Department of Transportation 49 CFR, Part 173.1300 Appendix A. Six rabbits (three males and three females; each 3-6 months in age) received 0.5 ml of 90.9% active material to the shaved intact skin. There were three intact skin test sites per animal. The first site was dosed, then washed and

observed three minutes later. A second site was dosed, occluded for one hour and then washed and observed. A third site was dosed, occluded for four hours and then washed and observed. All sites were observed again at 48 hours after dosing.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: Rhodacal 330 (formerly Siphonate 330; 91.4% active; Lot No. BA2K023949; viscous amber liquid (CAS #**90218-35-2**; Benzenesulfonic acid, dodecyl-, branched, compds with 2-propanamine).

Remarks: Tissue destruction (necrosis or ulceration) was not observed in any animals at any observation times.

Reference: **33.** Kuhn, J.O. Stillmeadow, Inc. Rhodacal 330: Skin Corrosion Study in Rabbits – DOT Guidelines; Study No. 0471-93 / PS-3230; October 20, 1993.

Reliability: 2 Valid with restrictions. Test substance [CAS RN] confirmed by sponsor at time of robust summary preparation, but not included in report.

CAS No. 68411-30-3

(a)

Species/strain: rabbit

Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**

Classification: Highly corrosive (causes severe burns) **[ ]**; Corrosive (causes burns) **[ ]**; Irritating **[X]**; Not irritating **[ ]**

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion" 1981. Three male and female rabbits received 0.5 ml of 50% active material to the shaved intact skin.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Marlon A 350 (CAS # **68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; activity: 50%.

Remarks: Mean irritation index: 5.1 out of 8. Individual scores: edema: 2.28, erythema: 3.0

Reference: **64.** Murmann, P. 1983a. Prufung der akuten Hautreizwirkung von Marlon A 350. Huels Report No. 0171.

Reliability: 2 Valid with restrictions

8.4.2.2 Eye Irritation/Corrosion

CAS No. 26264-05-1

(a)

Title Modified eye irritation

Date of report September 30, 1980.

GLP No data

Reference **23. Rhone-Poulenc.** 1980. Report T-1101. Product Safety Labs.
Test substance Benzenesulfonic acid, dodecyl-, compd. with isopropylamine (1:1), purity 90.9%.
Guideline EPA 40 CFR 163.81-4
Test system
Species Rabbit (New Zealand White).
No. of animals 3 (with rinsing) and 6 (without rinsing), sex not indicated.
Dosage Application of 0.1 ml test substance in the eye. For 3 animals eyes were rinsed with water 30 seconds after instillation.
Observation Observations at 24, 48 and 72 h and on day 4 and 7 after application.
Stat. method Not applicable.
Results

Test with rinsing

Animal	**1**				**2**				**3**			
Effect	C	I	Conj		C	I	Conj		C	I	Conj	
Time			Red	Ch			Red	Ch			Red	Ch
24 h	2	0	2	2	2	0	2	3	2	0	2	4
48 h	2	0	2	3	2	0	2	4	2	1	2	4
72 h	2	1	1	3	2	0	2	3	3	1	2	4
4 d	1	1	1	2	2	0	3	3	2	1	2	3
7 d	2	1	0	1	2	0	1	2	3	1	2	3

Test without rinsing

Animal	**1**				**2**				**3**				**4**				**5**				**6**			
Effect	C	I	Conj		C	I	Conj		C	I	Conj		C	I	Conj		C	I	Conj		C	I	Conj	
Time			Red	Ch			Red	Ch			Red	Ch			Red	Ch			Red	Ch			Red	Ch
24 h	3	1	2	3	2	0	2	4	2	1	2	4	2	0	2	4	2	0	2	3	3	0	0	4
48 h	3	1	2	3	2	0	1	4	3	0	1	4	2	0	1	3	2	0	2	3	2	0	1	4
72 h	3	1	2	4	2	0	1	4	4	2	1	4	2	1	1	2	2	0	2	4	2	1	1	3
4 d	3	0	2	1	2	0	1	2	2	1	1	3	1	0	1	0	1	1	2	3	2	1	1	1
7 d	3	0	1	3	3	1	1	3	3	1	0	3	2	0	0	0	2	1	1	2	3	1	1	2

C=corneal opacity I=Iris Conj=conjunctiva Red=redness Ch=chemosis

Conclusion Irritating
Reliability 2 Valid with restrictions. GLP not indicated.

CAS No. 26264-06-2

(a)
Title MSDS Rhodacal® CA/70
Date of August 17, 1999.

report
GLP No
Reference **21. Rhodia.** 1998. MSDS RHODOCAL®CA/70
Test substance Benzenesulfonic acid, dodecyl-,calcium salt, purity 69-71%.
Guideline Not specified.
Eye irritation Severely irritating in rabbit.
Reliability 4 Not assignable. Secondary literature

CAS No. 90218-35-2
(a)
Species/strain: rabbit / New Zealand Albino
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[X]**; Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**
Classification: Irritating **[X]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method: Modified Eye Irritation (Draize). EPA 40 CFR 163.81-4. Nine young adult rabbits dosed with 0.1 mL of test substance (90.9% active) in one eye. Eyes of three rabbits were irrigated with 20 mL of lukewarm water after 30 seconds. The eyes of the remaining six rabbits were not irrigated. Ocular lesions were evaluated at 24, 48 and 72 hours and at 4, 7 and 14 days after dosing. Temperature was maintained at 68-72^{o}F and photoperiod was a 12 hr light-dark cycle.
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Siphonate 330; alkyl aryl sulfonate 90.9% active; a clear brown-gold viscous liquid Lot #B949G9 (CAS #**90218-35-2**; Benzenesulfonic acid, dodecyl-, branched, compds with 2-propanamine).
Remarks: The MMTS of the test substance in the unwashed eye is 56.5. The MMTS of the test material in the washed eye is 52.7. Draize scores remained high through 7 days with the highest scores associated with the cornea
Reference: **34.** ALCOLAC, Inc (Rhodia) Product Safety Labs Test report No. T-1101 / PS-1764; Modified Eye Irritation; September 29, 1980.
Reliability: 2 Valid with restrictions (Test substance [CAS RN] confirmed by sponsor at time of robust summary preparation, but not included in report.)

CAS No. 68411-30-3
(a)
Species/strain: rabbit
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;

	Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**
Classification:	Irritating **[X]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion" 1981
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; activity: 50%.
Remarks:	The mean irritation index was 26.5 out of 110. Individual scores: 1.0; iris: 0; conjunctivae chemosis: 1.11, conjunctivae redness: 2.39
Reference:	**65.** Murmann, P. 1983b. Prufung der akuten Augen-und Schleimhautreiz Wirkung von Marlon A 350. Huels Report No. 0172.
Reliability:	2 Valid with restrictions
(b)	
Species/strain:	rabbit
Results:	Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**
Classification:	Irritating **[X]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method:	0.1 mL solutions of LAS at 5 different concentrations ranging from 0.01 to 1.0 % were instilled in the eyes of rabbits (13 per group). The rabbits were observed for 24 hours after LAS application.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	C_{10-13} LAS, (CAS #**68411-30-3**). Molecular weight 346.5; average alkyl chain length = $C_{11.9}$
Remarks:	Information as cited in IPCS document. The 0.01 % group showed no abnormalities, but the 0.05 % group showed slight congestion. The groups of 0.5 % and higher concentrations showed marked reactions such as severe congestion and oedema, increased secretion, turbidity of the cornea, and disappearance of corneal reflex.
Reference:	**66.** Oba, K., Mori, A. and Tomiyama, S. 1968. Biochemical studies of n-alpha-olefin sulfonates (II) Acute toxicity, skin and eye irritation, and some other physical properties. Journ. Jap. Oil Chem. Soc. 17:628-634. (In Japanese) cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.4.3 Skin Sensitization

CAS No. 68411-30-3

(a)

Type:	Guinea pig maximisation test
Species/strain:	guinea pig, females
Results:	Sensitising **[ ]**; Not sensitising **[X]**; Ambiguous **[ ]**
Classification:	Sensitising **[ ]**; Not sensitising **[X]**
Method:	OECD Guide-line 406 "Skin Sensitisation" 1981
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; activity: 50%.
Remarks:	0.1% intracutaneous and 3% epidermal doses. No sensitizing effects were observed.
Reference:	**67.** Murmann, P. 1988. Prufung auf hautsensibilisierende Wirkung am Meerschweinchen von Marlon A 350. Huels Report No. 1387.
Reliability:	2 Valid with restrictions

8.4.4 Repeated Dose Toxicity

CAS No. 27323-41-7

(a)

Title	Final report on the safety assessment of sodium dodecylbenzenesulfonate/TEA-dodecylbenzenesulfonate/sodiumdecylbenzenesulfonate	
Date of report	1997.	
GLP	No data	
Reference	**1. Cosmetic, Toiletry and Fragrance Association (CTFA).** 1997. CTFA Final report on Na/TEA DDBS.	
Test substance	Benzenesulfonic acid, dodecyl-, compd. With 2,2',2"-nitrilotris(ethanol)(1:1),0.5% a.i. in semipermanent hair dye	
Guideline	Not indicated.	
Stat. method	Not applicable.	
Test system	**Species**	Rabbit (New Zealand White).
	No. of animals	6/sex/dose group (3 control groups).
	Dosage	13 week-study with twice weekly dermal application of 1 ml/kg to the shaved skin (abraded in 3/sex/dose) with rinsing 1 hour after dosing.
	Observations	Body weight weekly. Clinical chemistry, haematology and urinalysis at initiation and after 3, 7 and 13 weeks. Necropsy in week 13 (macro- and microscopy).

Results	No treatment related effects. The significantly increased levels of BUN (all) and leukocyte count (males only) and decreased methaemaglobin level (females only) in treated animals were considered to be toxicologically irrelevant.
Conclusions	NOAEL > 0.005 ml/kg bw (equivalent to 5 mg/kg bw); only dose tested
Reliability	2 Valid with restriction - CTFA Cosmetic Ingredient Review

CAS No. 42615-29-2
(a)

Title	Toxicology Studies of Linear Alkylbenzene Sulphonate (LAS) in Rhesus Monkeys I. Simultaneous Oral and Subcutaneous Administration for 28 Days	
Date of report	1978.	
GLP	No.	
Reference	**5. Heywood R., James R., Sortwell R.** 1978. Toxicology studies of linear alkylbenzene sulphonate (LAS) in rhesus monkeys I. Simultaneous oral and subcutaneous administration for 28 days. Toxicol 11: 245-250	
Test substance	Benzenesulphonic acid, linear alkyl, purity 20.5% (78.7% water)	
Guideline	Not indicated.	
Stat. method	Not indicated.	
Test system	**Species**	Rhesus Monkey (*Macaca mulatta*), 2.0-4.4 kg, age 18-36 months.
	No. of animals	3/sex/treatment.
	Dosage	Simultaneous oral (gavage) and subcutaneous administration of 30 p.o./0.1 s.c., 150 p.o./0.5 s.c. and 300 p.o./1.0 s.c. mg/kg during 28 days; dose volume 4 ml/kg (p.o.) and 0.17 ml/kg (s.c.); vehicle (water) controls.
	Observation	As per OECD 407 with the exception of some clinical chemical parameters (cholesterol, albumine and creatinine).

Results

Dose (mg/kg bw)	**0/0**	**30/0.1**	**150/0.5**	**300/1.0**	**DR**
Mortality		None			
Clinical signs- systemic[(A)]			+	+	x
- local[(B)]		+	+	+	x

Body weight gain/food consumption	No treatment related effects	
Ophthalmoscopy	No treatment related effects	
Blood parameters/urine analysis	No treatment related effects	
Organ weights	No treatment related effects	
Macroscopy/histopathology	No treatment related effects	

(A) Vomiting (~3 h after application) and abnormal faeces.
(B) Chronic inflammatory cell infiltration (mainly fibroblasts) at the injection site associated with pseudocysts, haemorrhage and necrosis.

Conclusions NOAEL = 301 mg/kg ⇔ 60 mg a.i./kg.

Rev. note
1. Clinical signs were treatment related but not considered to be significantly adverse.
2. Most probably no statistical evaluation of the results was performed in view of the low number of animals in this study.

Reliability 2 Valid with restrictions. Non-GLP study

(b)

Title Ultrastructural observations of the protective effect of glycyrrhizin for mouse liver injury caused by oral administration of detergent ingredient (LAS)

Date of report 1977.

GLP No.

Reference **30. Wateri N., Torizawa K., Kanai M., Suzuki Y.** 1977. Ultrastructural Observations of the Protective Effect of Glycyrrhizin for Mouse Liver Injury Caused by Oral Administration of Detergent Ingredient (LAS). J. Clin. Electron Microsc. 10: 121-139

Test substance Benzenesulphonic acid, linear alkyl

Guideline Not indicated.

Stat. method Not indicated.

Test system

Species Mouse (DDY-strain).

No. of animals Not indicated.

Dosage Administration for 6 months at 0 and 100 ppm in drinking water with 2 months recovery ⇔ males: 0 and 17 mg/kg bw, females: 0 and 20 mg/kg bw.

Observations Microscopical examination (electron microscope) of liver tissues of animals sacrified at 1, 2, 3, 6 and 8 months after study initiation.

Results Hypofunctional and injured liver cells with disappeared nucleolonema, atrophic Golgi apparatus, degranulation of RER and mitochondria and increased number of lysosomes with autophagic vacuoles. After the recovery period mitochondria were still altered and in some hepatic cells fatty metamorphosis was observed.

Conclusions Liver effects at 17 mg/kg bw.

Rev. note
1. No information on accuracy of preparation, stability and homogeneity was provided. The actual test substance intake was calculated by the reviewer from estimated water intake of 5 ml/day and a mean bodyweight 30 g for males and 25 g for females.
2. The information in this journal article was limited to the above-mentioned.
3. The identity of the test substance could not be established.

Reliability 4 Not assignable. Limited report and no confirmation of test substance.

CAS No. 68411-30-3

(a)

Species/strain:	Rat/Sprague-Dawley
Sex:	Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration:	gavage
Exposure period:	one month
Frequency of treatment:	.....daily
Dose:	125, 250, 500 mg/kg bw d.
Control group:	Yes **[X]**; No **[ ]**; No data **[ ]**; Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[]**
NOAEL:	125 mg/kg bw d
LOAEL:	250 mg/kg bw d
Results:	Diarrhea was observed in the 500 mg/kg group and soft stools were observed in the other 2 groups. Body weight gain was suppressed in all the male groups and in the female 500 mg/kg group. Haematological examinations revealed no abnormalities. Serum-biochemical examinations revealed several differences among the mid and high dose group compared to the control group. The weight of the spleen and the heart significantly decreased in the male high dose group. In the female high dose group, the weight of the liver increased while the weight of the heart and thymus decreased. Histological findings of the liver revealed no abnormalities.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Remarks:	Information as cited in IPCS document. 12 animals / dose group.
Test substance:	..... C_{10-13} LAS, sodium salt (CAS #**68411-30-3**) <C_{10} 0.1%, C_{10} 10.1%, C_{11} 33.7%, C_{12} 31.0%, C_{13} 25.1%; average alkyl chain length = $C_{11.7}$; activity: 99.5%
Reference:	**68.** European Commission. 2000. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. IUCLID Year 2000 CD-ROM edition.

63. Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M. and Fukushima, A. 1978. J. Med. Soc. Toho, Japan, 25:850-875 (in Japanese). cited in IPCS. 1996. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates and Related Compounds. World Health Organization, Geneva, Switzerland.

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

(b)

Species/strain: mouse (ICR)

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**

Administration: Oral feed or water

Exposure period: 9 months

Frequency of treatment: Daily

Dose: Diet: 0.6 and 1.8% (corresponding to 500 and 1000 mg/kg bw d).

Diet: Drinking water: 0.07, 0.2, and 0.6% (100, 250, and 600 mg/kg bw d for males and 100, 250, and 900 mg/kg bw d for females)

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[]**

NOAEL: 250 mg/kg bw d in drinking water

LOAEL: 500 mg/kg bw d in diet

Results: In the mice given 0.6% in their diet, body weight gain was not suppressed, but the weight of the liver increased in male and female mice. Enzymatic examinations revealed significant decreases in LDH of the liver and in acid phosphatase of the kidneys in the male mice. For mice given LAS in drinking water, body weight was depressed at the highest dose for males and females. This dose also elicited an increase in liver weight in females and significant decreases in renal Na and K-ATPase.

Method: Groups of 8 or 9 mice were given diets containing LAS at concentrations of 0.6 and 1.8% or drinking water containing LAS at concentrations of 0.07, 0.2, and 0.6% for 9 months.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS

Reference: **68.** European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.

69. Yoneyama, M., Mabuchi, Y., Ikawa, M., Kobayashi, H. and Ichikawa, H. 1976. Subacute toxicity of linear alkylbenzene sulfonate. Ann. Rep. Tokyo Metr. Res. Lab. P.H. 27(2):105-112 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

42. HERA. 2004. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No.

68411-30-3, Version 2.0 June 2004.
http://www.heraproject.com/riskassessment.cfm. .

Reliability: 2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.4.5 Genetic Toxicity *In Vitro*

8.4.5.1 Bacterial Test

CAS No. 42615-29-2

(a)

Title	Studies of *in vitro* cell transformation and mutagenicity by surfactants and other compounds	
Date of report	1979.	
GLP	No	
Reference	**6. Inoue K., Sunakawa T.** 1980. Studies of *in vitro* cell transformation and mutagenicity by surfactants and other compounds. Food Cosmet Toxicol 18: 289-296	
Test substance	Benzenesulphonic acid, linear alkyl, C_{10} -C_{14}, purity 22% active (0.033% alkylbenzene, 0.02% $NaSO_4$).	
Guideline	Not indicated	
Stat. method	Not indicated.	
Test system	**Bacterial strains**	TA98, TA100.
	Metabolic activation	Rat liver S9 mix (polychlorinated biphenyl-induced).
	Test concentration	10, 25, 50, 100 and 200 µg/plate.
	Controls	Negative: vehicle (DMSO or water not specified). Positive: 4-nitroquinoline 1 oxide, *N*-methyl-*N*'-nitro-*N*-nitrosoguanidine, benzo[a]pyrene, 2-acetylaminofluorene, *N*-nitrosomethylamine.
	Procedure	According to OECD 471.

Results

Tester strain	**Test result[(A)]**	
	Without activation	**With activation**
TA98	-	-
TA100	-	-

(A) +/- : positive/negative result; positive controls gave expected responses.

Conclusion Not mutagenic.
Rev. note Secondary literature.
Reliability 2 Valid with restrictions. Secondary literature, non-GLP study.

CAS No. 68411-30-3

(a)

Type:	Ames test
System of testing:	*Salmonella typhimurium* TA 1535, TA 1537, TA 1538, TA 98, TA 100
Concentration:	8 -5000 ug/plate
Metabolic activation:	With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:	
Cytotoxicity conc:	With metabolic activation: > 5000 μg/plate
	Without metabolic activation: > 5000 μg/plate
Genotoxic effects:	+ ? -
	With metabolic activation: **[ ] [ ] [X]**
	Without metabolic activation: **[ ] [ ] [X]**
Method:	Directive 84/449/EEC, B.14 Mutagenicity (*Salmonella typhimurium* - reverse mutation assay)" 1984
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	Marlon A 390 (CAS #**68411-30-3**) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; activity 91.3%
Remarks:	Negative and positive controls used.
Reference:	**70.** Schoeberl, P. 1993. Bestimmung der Mutagenitat von Marlon A 390 im Salmonella/Sauger-Mikrosomen-Mutagenitatstest nach Ames. Huels Final Report No. AM-93/12.
Reliability:	1 Valid without restriction

8.4.5.2 Non-Bacterial Test

CAS No. 42615-29-2

(a)

Title	Studies of *in vitro* cell transformation and mutagenicity by surfactants and other compounds	
Date of report	1979.	
GLP	No.	
Reference	**6. Inoue K., Sunakawa T.** 1980. Studies of *in vitro* cell transformation and mutagenicity by surfactants and other compounds. Food Cosmet Toxicol 18: 289-296	
Test substance	Benzenesulphonic acid, linear alkyl, C_{10} -C_{14}, purity 22% active (0.033% alkylbenzene, 0.02% $NaSO_4$).	
Guideline	Not indicated.	
Stat. method	Not indicated.	
Test system	**Cell culture**	Syrian golden hamster embryo cells.
	Test concentration	5, 10, 20 and 50 μg/ml. 0.5, 1, 5 and 10 μg/ml.
	Controls	Negative: vehicle (DMSO).

Positive: 3-methylcholanthrene

Procedure Pregnant Syrian golden hamsters were killed on day 13 or 14 of gestation. Embryos were minced and trypsinised and cells were cryopreserved. Unthawed cells were plated twice (as feeder-layer and target cells) on day 0 and 3 resp.. On day 4 feeder-layer cells were plated (after irridiation and trypsination) at $6x10^4$ cells/dish and on day 5 500 target cells/dish were added to the dishes. On day 6 the test substance was added. On day 14 cultures were fixed and stained and normal and transformed colonies were counted.

Results Positive control negative.

Doses tested [μg/ml]	**Cytotoxicity [% of control survival] at highest dose**	**Test result(A)**
5, 10, 20, 50	40%	-
0.5, 1, 5, 10	88%	-

(A) +/- : positive/negative result.

Conclusion Not mutagenic.

Rev. note 1. The results of a simultaneously performed test with the positive control (at 0.1, 0.5 and 1.0 μg/ml) were negative. This lowers the value of the assay

Reliability 4 Not assignable. Positive control was negative.

CAS No. 68411-30-3

(a)

Type:	Micronucleus assay
Species/strain:	mouse (ddy)
Sex:	Male
Administration:	intraperitoneal injection
Exposure Period:	single dose
Doses:	100 mg/kg bw
Results:	There were no differences in the incidences of polychromatic erythrocytes with micronuclei in the bone marrow cells between the treated group and the control group.
Method:	Three male mice were each given a single i.p. injection of 100 mg/kg bw LAS.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Benzenesulfonic acid, C10-13 alkyl derivatives; sodium salts.
Remarks:	Information as cited in the IPCS document.
Reference:	**73.** Kishi, M., Satoh, S., Horiguchi, Y. and Ito, K. 1984. Effects of surfactants on bone marrow cells. Bull. Kanagaw Public Health Lab. 14:57-58. as cited in 1996 IPCS Environmental Heath Criteria

	169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability:	2 Valid with restrictions. Original study reports were not obtained but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

8.4.6 Toxicity to Fertility

8.4.6.1 Developmental Toxicity

CAS No. 27323-41-7

(a)

Title	Final report on the safety assessment of sodium dodecylbenzenesulfonate/TEA-dodecylbenzenesulfonate/sodiumdecylbenzenesulfonate	
Date of report	1997.	
GLP	No data	
Reference	**1. Cosmetic, Toiletry and Fragrance Association (CTFA).** 1997. CTFA Final report on Na/TEA DDBS.	
Test substance	Benzenesulfonic acid, dodecyl-, compd. with 2,2',2"-nitrilotris(ethanol) (1:1), 0.5% a.i. in semipermanent hair dye.	
Guideline	Not indicated.	
Stat method	Not applicable.	
Test system	**Species**	Rat (CD).
	No. of animals	20 females/dose group (3 control groups).
	Dosage	Dermal application of 2 ml/kg to the shaved skin on day 1, 4, 7, 10, 13, 16 and 19 of gestation.
	Observations	Necropsy on day 20 and examination of foeteuses
Results	No treatment related effects.	
Conclusions	NOAEL > 0.01 ml/kg bw (equivalent to 10 mg/kg bw); only dose tested	
Reliability	2 Valid with restriction - CTFA Cosmetic Ingredient Review.	

CAS No. 42615-29-2

(a)

Title	A Teratology Study of Topically Applied Linear Alkylbenzene Sulphonate in Rats
Date of report	1980.
GLP	No data
Reference	**2. Daly I., Schroeder R., Killeen J.** 1980. LAS teratology study in rats. Food Cosmet Toxicol 18: 55-58
Test substance	Benzenesulphonic acid, linear alkyl, purity 20.5% (0.2% alkylbenzene, 0.6% ash, 78.7% water).
Guideline	Not indicated.

Stat. method	*F*-test, Student's *t*-test (when applicable chi-square). Test groups were compared with water treated controls.	
Test system	**Species**	Rat (Wistar), age 12-18 weeks.
	No. of animals	20-21 mated females/treatment.
	Dosage	Dermal application of 1, 2, 10, 20, 100 and 400 mg/kg bw (0.5 ml in tap water) on the clipped skin (24 cm^2,10% of body surface); unclipped, clipped but not treated and clipped water treated controls; at 20, 100 and 400 mg/kg the test substance was washed off with water after 30 min.
	Procedures	Female rats were mated with untreated males (1/1) from the same strain. The day of observation of sperm was defined as day 0 of gestation. Females were treated daily from day 0 to 20 of gestation inclusive. Body weight, food consumption and clinical signs were recorded daily. All females were subjected to macroscopic examination on day 21. The uteri were removed and examined for no. of corpora lutea, no. of implantation sites and no. and location of foetuses and resorptions. Foetuses were inspected on total number, viability, sex, weight and external, visceral and neural (½ of foetuses) and skeletal (½ of foetuses) defects. The number of vertebrae and phalanges was recorded.

Results

Dose (mg/kg bw)	**0 (unclipped)**	**0 (clipped)**	**0 (veh)**	**1**	**2**	**10**	**20**	**100**	**400**	**DR**
Maternal data										
Mortality	None									
Clinical signs [(A)]							+	+	+	x
Mean body weight day 12-21									d (5%)	
Food intake	No treatment related effects									
Necropsy	Not reported									
No. of pregnant females	20/20	20/20	20/20	19/20	20/20	20/20	20/20	20/20	20/21	
No. of corpora lutea and implantation sites /dam	No treatment related effects									
Implantation loss/ resorptions	No treatment related effects									
No. live foetuses/ dam	No treatment related effects									
Foetal data										
No. of litters included in evaluations	19	20	20	19	20	20	20	20	20	

Foetal weight / sex	No treatment related effects	
External,visceral/neural/ Skeletal examination	No treatment related effects	
No. vertebrae and phalanges	No treatment related effects	

(A)Discolouration ((light) brown), erythema, fissuring and slight thickening of the skin. Reported as "marked" at 400, "slight" at 100, and discolouration only at 20.

Conclusions "This study demonstrated that LAS is free of teratogenic and embrypathic effects when applied to the dermis of pregnant Wistar rats at concentrations that elicit marked skin changes and reductions in maternal body weight.
NOAEL for maternal toxicity: 100 mg/kg bw⇔ 20.1 mg a.i./kg bw (based on 5% weight loss).
NOAEL for reproductive effects: 400 mg/kg bw ⇔ 82 mg a.i./kg bw.

Rev. note
1. The test substance was only applied for 30 minutes daily for 20, 100 and 400 mg/kg bw dose groups.
2. Clinical signs were treatment related but not considered toxicologically significant.

Reliability 2 Valid with restriction - Non-GLP study

(b)

Title Assessment of the teratogenic potential of surfactants Part 1 – LAS, AS and CLD

Date of report 1975.

GLP No.

Reference **18. Palmer A., Readshaw M., Neuff A.** 1975. Assessment of the teratogenic potential of surfactants part I LAS AS and ClD. Toxicol. 3: 91-106

Test substance Benzenesulphonic acid, linear alkyl), purity not indicated.

Guideline Not indicated.

Stat. method Wilcoxon-test.

Test system

Species Rabbit (New Zealand White), rat (CD) and mouse (CD-1).

No. of animals 20 females/treatment (13 for rabbits).

Dosage Administration by oral gavage at 0.2, 2.0, 300 and 600 mg/kg bw (vehicle: water); vehicle treated controls; solutions were prepared daily.

Procedures Females were mated. The day of observation of a vaginal plug (rats and mice) or observation of coitus (rabbit) was defined as day 0 of gestation. Females were treated daily

from day 6 to 15 (18 for rabbits) of gestation. Mortality/clinical symptoms of dams were noted daily. Body weight was recorded regularly. All females were subjected to macroscopic examination day 17, 20 and 29 for mice, rats and rabbits, respectively, or on day of death. The uteri were removed and examined for no. of corpora lutea, no. of implantation sites and no. of foetuses and resorptions. Foetuses were inspected on total number, sex, weight and external, visceral (1/3 of foetuses in rats and mice,all in rabbits) and skeletal (2/3 of foetuses in rats and mice,all in rabbits) defects.

Results Mice

Dose (mg/kg bw)	**0**	**0.2**	**2.0**	**300**	**600**	**DR**
Maternal data						
Mortality	0/20	0/20	0/20	7/20	18/20	x
Clinical signs (A)				+	+	
Body weight gain				d	d	x
Necropsy	Not reported					
No. of pregnant females	17/20	18/20	18/20	20/20	19/20	
No. of implantation sites /dam	No treatment related effects					
Pre-implantation loss	Not reported					
Post-implantation loss/ resorptions					i	
No. live foetuses/ dam				dc	N/A	x
Foetal data						
No. of litters included in evaluations	17	18	18	9	N/A	
Foetal weight		ic			N/A	
External examination / sex	No treatment related effects				N/A	
Anomalies: visceral/ skeletal (B)				i	N/A	

(A) Disturbance of the gastro-intestinal tract.
(B) No details provided.

Results Rats

Dose (mg/kg bw)	**0**	**0.2**	**2.0**	**300**	**600**	**DR**
Maternal data						
Mortality	0/20	0/20	0/20	0/20	1/20	
Clinical signs (A)					+	
Body weight gain					d	
Necropsy	Not reported					
No. of pregnant females	15/20	15/20	18/20	16/20	17/20	
No. of corpora lutea / implantation sites per dam	No treatment related effects					
Pre/post-implantation loss/ resorptions	No treatment related effects					
No. live foetuses/ dam	No treatment related effects					

Foetal data						
No. of litters included in evaluations	15	14	18	16	16	
Foetal weight		ic	ic			
External examination / sex		No treatment related effects				
Anomalies: visceral/ skeletal		No treatment related effects				

(A)Disturbance of the gastro-intestinal tract.

Results Rabbits

Dose (mg/kg bw)	**0**	**0.2**	**2.0**	**300**	**600**	**DR**
Maternal data						
Mortality	2/13	0/13	1/13	11/13	13/13	x
Clinical signs [(A)]				+	+	
Body weight gain				d	d	x
Necropsy			Not reported			
No. of pregnant females	12/13	13/13	12/13	2/13	0/13	
No. of corpora lutea /implantation sitesper dam		No treatment related effects			N/A	
Pre-implantation loss			No treatment related effects			
Post-implantation loss/ resorptions				i	N/A	
No. live foetuses/ dam				dc	N/A	x
Foetal data						
No. of litters included in evaluations	9	12	11	2	N/A	
Foetal weight		No treatment related effects		N/A	N/A	
External examination / sex		No treatment related effects		N/A	N/A	
Anomalies: visceral/ skeletal [(B)]		No treatment related effects		N/A	N/A	

(A)Diarrhoea, anorexia and cachexia were seen among animals.

Conclusions "Effects on litter parameters were generally restricted to dosages causing marked maternal toxicity, the principal effects being higher foetal loss (with consequent reduction in litter size) arising from the increased incidence of total litter loss. When dams showing total litter loss were excluded from the calculations, litter parameters were not unduly different from those of controls. At dosages that were either non-toxic or only slightly to moderately toxic to the dam, litter parameters were essentially unaffected."
NOAEL for maternal toxicity: > 2 but <300 mg/kg for mice and rabbits; 300 mg/kg for rats.
There were no teratogenic and embryotoxic effects observed at any dose level.

Rev. note 1. Limited information was available on the identity of the test

substance. It was assumed by the reviewer that the test substance was the benzenesulphonic acid, linear alkyl.

2. Effects on reproduction were seen at doses exhibiting maternal toxicity.
3. Anomalies reported in foetuses and sex of the foetuses were not identified.
4. Large (>100 X) gap in doses between NOAEL and LOAEL for maternal toxicity for mice and rabbits makes it difficult to establish a true NOAEL.

Reliability 2 Valid with restrictions

(c)

Title	Assessment of the teratogenic potential of surfactants Part III – Dermal application of LAS and Soap	
Date of report	1975.	
GLP	No.	
Reference	**19. Palmer A., Readshaw M., Neuff A.** 1975. Assessment of the teratogenic potential of surfactants part III- dermal application of LAS and soap. Toxicol 4: 171-181	
Test substance	Benzenesulphonic acid, linear alkyl, purity not indicated.	
Guideline	Not indicated.	
Stat. method	Wilcoxon-test.	
Test system	**Species**	Rabbit (New Zealand White), rat (CD) and mouse (CD-1).
	No. of animals	20 females/treatment (13 for rabbits).
	Dosage	Dermal application of 0.03, 0.30 and 3.00% solutions (vehicle: water) to 240, 16 and 6 cm^2 for rabbits, rats and mice resp.(dosing volume 0.5 (rat, mouse) or 10 ml (rabbit)); vehicle treated controls; solutions were prepared daily; application in two parts (with drying period, no occlusion).
	Procedures	Females were mated. The day of observation of a vaginal plug (rats and mice) or observation of coitus (rabbit) was defined as day 0 of gestation. Females were treated daily from day 2 to 15 (rats), 2 to 13 (mice) and 1-16 (rabbits) of gestation. Mortality/clinical symptoms of dams were noted daily. Body weight was recorded regularly. All females were subjected to macroscopic examination day 17, 20 and 29 for mice, rats and rabbits resp. or on day of death. The uteri were removed and examined for no. of

corpora lutea, no. of implantation sites and no. of foetuses and resorptions. Foetuses were inspected on total number, sex, weight and external, visceral (1/3 of foetuses in rats and mice,all in rabbits) and skeletal (2/3 of foetuses in rats and mice,all in rabbits) defects.

Results Mice

Dose (%)	**0**	**0.03**	**0.3**	**3**	**D R**
Dose (mg/kg bw)	**0**	**5**	**50**	**500**	
Maternal data					
Mortality	1/20	1/20	0/20	0/20	
Clinical signs (A)			+	+	x
Body weight gain				d	
Necropsy	Not reported				
No. of pregnant females	17/20	16/20	18/20	6/20	
No. of implantation sites /dam	No treatment related effects				
Post-implantation loss/ resorptions			i	i	x
No. live foetuses/ dam				d	
Foetal data					
No. of litters included in evaluations	14	15	14	1	
Foetal weight	No treatment related effects				
External examination	No treatment related effects			N/A	
Anomalies: visceral/ skeletal (B)				i	

(A)Erythema, oedema (peak on day 6, dead skin), irritability and hypersensitivity were seen among animals. Effects were reversible

(B)No visceral examination of foetuses of high dosed females. Skeletal examinations revealed extra ribs (cervical).

Results Rats

Dose (%)	**0**	**0.03**	**0.3**	**3**	**D R**
Dose (mg/kg bw)	**0**	**0.6**	**6**	**60**	
Maternal data					
Mortality	None				
Clinical signs (A)				+	
Body weight gain	No treatment related effects				
Necropsy	Not reported				
No. of pregnant females	20/20	18/20	20/20	18/20	
No. of corpera lutea / implantation sites per dam	No treatment related effects				
Pre/post-implantation loss/ resorptions	No treatment related effects				
No. live foetuses/ dam	No treatment related effects				
Foetal data					
No. of litters included in evaluations	19	18	20	18	
Foetal weight				ic	

External examination	No treatment related effects	
Anomalies: visceral/ skeletal	No treatment related effects	

(A) Erythema, oedema (peak on day 4-5), irritability and hypersensitivity were seen among animals. Effects were reversible.

Results Rabbits

Dose (%)	**0**	**0.03**	**0.3**	**3**	**D R**
Dose (mg/kg bw)	**0**	**0.9**	**9**	**90**	
Maternal data					
Mortality	0/13	0/13	1/13	0/13	
Clinical signs [(A)]			+	+	
Body weight gain			d	d	
Necropsy	Not reported				
No. of pregnant females	12/13	12/13	13/13	11/13	
No. of corpera lutea / implantation sites per dam	No treatment related effects				
Pre/post-implantation loss/ resorptions				i	
No. live foetuses/ dam				d	
Foetal data					
No. of litters included in evaluations	11	12	12	9	
Foetal weight	No treatment related effects				
External examination	No treatment related effects				
Anomalies: visceral/ skeletal	No treatment related effects				

(A) Erythema, oedema (peak on day 6-7, cracking and bleeding skin), irritability and hypersensitivity were seen among animals.

Conclusions "Effects on litter parameters were generally restricted to dosages causing marked maternal toxicity in mice, the principal effects being higher foetal loss (with consequent reduction in viable litter size) arising from an increased incidence of total litter losses. When dams showing total litter loss were excluded from the calculations, litter parameters were not unduly different from those of controls. Although LAS at 3% was considered to show marked maternal toxicity in the rabbit, the slightly higher foetal loss and lower litter size did not differ significantly from control values. The moderate maternal toxicity of LAS, 0.3% in the mouse correlated with a higher incidence of embryonic deaths and lower litter size but only the former differed significantly from the corresponding control value. At dosages that were non-toxic or only slightly toxic to the dam, litter parameters were not adversely affected… The incidence of major malformations, minor visceral or skeletal anomalies, and skeletal variants provided no conclusive evidence of specific teratogenicity even at maternally toxic dosages."
NOAEL for maternal toxicity: 0.3% = 50 mg/kg bw (mice), 0.3% = 9

	mg/kg bw (rabbits) and 3% = 60 mg/kg bw (rats) NOAEL for teratogenic and embryotoxic effects: no effects at any dose level
Rev. note	1. Effects on reproduction were seen at doses exhibiting maternal toxicity 2. Limited information was available on the identity of the test substance. It was assumed by the reviewer that the test substance was the benzenesulphonic acid, linear alkyl. 3. Clinical signs were treatment related but not considered toxicologically significant.
Reliability	2 Valid with restrictions.

CAS No. 68584-26-9

(a)

Title	LAS-Mg : Effects of oral administration upon the progress and outcome of pregnancy in the rabbit	
Date of report	December 21, 1978.	
GLP	No.	
Reference	**26. Tesh J.M. & Ross F.W.** 1978. LAS-Mg: Effects of oral administration upon the progress and outcome of pregnancy in the rabbit. Life Science research, Stock, Essex, UK	
Test substance	Magnesium salt of LAS, purity not indicated.	
Guideline	Not indicated.	
Stat. method	Not indicated.	
Test system	**Species**	Rabbit (New Zealand White), body weight 2730-5200 g.
	No. of animals	14 females/treatment.
	Dosage	Oral administration of 0, 60, 125 and 250 mg/kg bw (vehicle water) during day 6 to 18 of gestation; dosage volume 5 mL.
	Procedures	Females were mated with fertile males and injected with luteinising hormone on day 0 of gestation. Mortality and clinical signs of dams were noted daily. Body weights were recorded on day 0, 6, 8, 10, 12, 14, 16, 18, 23 and 28 of gestation. Food/water consumption was recorded on day 0, 5, 11, 17, 22 and 28. All females were killed on day 29 of gestation and subjected to macroscopic examination. The reproductive tract (incl. Ovaries) was dissected and examined for number of corpora lutea, implantations, early and late resorptions and foetuses. Foetuses were weighed, sexed and examined for external and skeletal abnormalities. Placenta weights were determined.

Results

Dose (mg/kg bw)	**0**	**60**	**125**	**250**	**DR**
Maternal					
Mortality	1/14	1/14	2/14	0/14	
Clinical signs	Not reported				
Body weight gain		d	d	d	X
Food/water consumption (day 6-17)		d	d	d	X
Macroscopy	No treatment related effects				
Number of pregnancies	10	14	12	13	
Corpora lutea/implantation sites	No treatment related effects				
Post implantation loss			i	i	X
Resorptions early	No treatment related effects				
Late				i	X
Placental weight				i	X
Foetal					
Number of litters evaluated	10	13	12	11	
Number of live foetuses			d	d	X
Weight/sex	No treatment related effects				
External/Skeletal abnormalities	No treatment related effects				

Conclusions "It was concluded from this investigation that LAS-Mg, administered to pregnant rabbits at dosages up to 250 mg/kg/day, had no adverse effects upon foetal morphology, although at dosages of 125 or 250 mg/kg/day survival in-utero was impaired. At dosages of 60 mg/kg day or above, there was some impairment of maternal economy, but no effects upon the foetus."
NOAEL for maternal effects = 60 mg/kg bw based on post implantation loss.
Effects on reproduction were observed at doses exhibiting maternal toxicity.
No teratogenicity or embryotoxicity were observed at any dose level.

Rev. note
1. The purity of the test substance is not indicated; therefore, a.i. dose could not be calculated.
2. No visceral examination of foetuses was performed.

Reliability 2 Valid with restrictions

(b)

Title LAS-Mg : Effects upon the progress and outcome of pregnancy in the rabbit

Date of report August 31, 1978.

GLP No.

Reference **27. Tesh J.M., Ross F.W. & Moss A.** 1978. LAS-Mg: Effects upon the

progress and outcome of pregnancy in the rabbit. Life Science research, Stock, Essex, UK

Test substance Magnesium salt of LAS, purity not indicated.

Guideline Not indicated.

Stat. method Not indicated.

Test system

Species Rabbit (New Zealand White), mean body weight 3800-4100 g.

No. of animals 14 females/treatment.

Dosage Topical application of 0, 0.75, 1.5 and 3.0% in PEG (3% aqueous) during day 6 to 18 of gestation; application volume 5 mL, application area 100 cm^2.

Procedures Females were mated with fertile males and injected with luteinising hormone on day 0 of gestation. Body weights were recorded on day 0, 6, 8, 10, 12, 14, 16, 18, 23 and 28 of gestation. Food/water consumption was recorded on day 0, 5, 11, 17, 22 and 28. All females were killed on day 29 of gestation and subjected to macroscopic examination. The reproductive tract (incl. ovaries) was dissected and examined for number of corpora lutea, implantations, early and late resorptions and foetuses. Foetuses were weighed, sexed and examined for external and skeletal abnormalities. Placenta weights were determined.

Results

Dose (%)	**0**	**0.75**	**1.5**	**3.0**	**DR**
Maternal					
Mortality			1/14	1/14	
Clinical signs (A)	+	+	+	+	X
Body weight (gain)	No treatment related effects				
Food/water consumption	No treatment related effects				
Macroscopy	No treatment related effects				
Number of pregnancies	14	13	12	11	
Corpora lutea/implantation sites	No treatment related effects				
Resorptions	No treatment related effects				
Placental weight	No treatment related effects				
Foetal					
Number of litters evaluated	14	11	11	11	
Number of live foetuses	No treatment related effects				
Weight/sex	No treatment related effects				
External/Skeletal abnormalities	No treatment related effects				

(A) Erythema and hyperkeratinisation.

Conclusions NOAEL for maternal effects 3%. Clinical signs were observed but not considered toxicologically significant.
NOAEL for reproductive effects 3%.

Rev. note
1. The application area was less than 10% of the body surface.
2. No information on the use of a (semi)occlusive dressing was available. If no dressing is used, some oral intake of the test substance can not be fully excluded.
3. The purity of the test substance is not indicated. Therefore the actual amount (a.i.) applied can not be calculated.
4. No visceral examination of foetuses was performed.

Reliability 2 Valid with restrictions

(c)

Title	LAS-Mg : The effects of topical application upon reproduction : Segment II study	
Date of report	January 9, 1979.	
GLP	No.	
Reference	**28. Tesh J.M., Wilson S.M. & Tesh S.A.** 1979. LAS-Mg: The effects of topical application upon reproduction: segment II study. Life Science research, Stock, Essex, UK	
Test substance	Magnesium salt of LAS, purity not indicated.	
Guideline	Guidelines of Japanese Ministry of Health and Welfare.	
Stat. method	ANOVA.	
Test system	**Species**	Rat (CD), 12 weeks old, weight 242-298 g.
	No. of animals	32 females/dose level.
	Dosage	Application of 0, 1.75, 3.5 and 7.0% test substance in 3%PEG to the clipped dorsal skin (area 32 cm^2) of F0 females; vehicle treated controls.
	Procedures	F0: Female rats were mated with untreated males (1/1) from the same strain. The day of observation of sperm or a copulatory plug was defined as day 0 of gestation. Females were treated daily from day 7 to 17 of gestation inclusive. Two-thirds of the females were sacrified on day 20 of gestation, the remaining females were allowed to deliver and their off-spring was observed for at least 8 weeks after parturition. F1: Selected off-spring from dams of the same treatment

group was allowed to mate (22/sex/group, 1/1) at the age of ten weeks. The day of observation of sperm or a copulatory plug was defined as day 0 of gestation. On day 20 of gestation the females were sacrified.

Observation

Maternal (F0)

- Mortality/clinical signs.
- Body weight on day 0, 2, 7, 9, 11, 13, 15, 17 and 20 of gestation.
- Food and water intake twice weekly.

Teratology (F0)

- No. of corpora lutea.
- No. of implantation sites.
- No. and location of foetuses and resorptions.

Foetuses (F1)

- Total number.
- Sex, weight.
- External, visceral (½ of foetuses) and skeletal (½ of foetuses) defects.

Post-natal (F0)

- Body weight twice weekly until weaning.
- Gestation duration, parturation.
- Macroscopy.

Young (F1)

- No., sex, weight.
- Viability/abnormalities.
- Postnatal development (physical/behavioural).
- Macroscopy.

Reproduction (F1)

- No. of corpora lutea.
- No. of implantation sites.
- No. and location of foetuses and resorptions.
- Macroscopy (males and females).

Foetuses (F2)

- Total number.
- Sex, weight.
- External defects.

Results

Dose (%)	**0**	**1.75**	**3.5**	**7.0**	**DR**
F0 (prenatal)					
Mortality	None				
Clinical signs [(A)]		+	+	+	X
Body weight (gestation)				d	

Food/water consumption [(B)]	No treatment related effects				
Macroscopy[(C)]	No treatment related effects				
Non-pregnant females	0/32	1/32	0/32	0/32	
Corpora lutea/implantation sites	No treatment related effects				
Implantation loss/resorptions	No treatment related effects				
Foetal evaluation (F1)					
Number of litters evaluated	11	11	11	11	
Number of live foetuses	No treatment related effects				
Weight/sex	No treatment related effects				
External[(D)]/Skeletal/visceral abnormalities	No treatment related effects				
F0 (postnatal)					
Mortality/clinical signs	No treatment related effects				
Body weight (lactation)	No treatment related effects				
Gestation time/parturation	No treatment related effects				
Evaluation of offspring (F1)					
Number of viable young	No treatment related effects				
Body weight[(E)]				d	
Sex	No treatment related effects				
Postnatal development	No treatment related effects				
Macroscopy	No treatment related effects				
F1 (prenatal)					
Mortality			1 male		
Clinical signs	No treatment related effects				
Body weight	No treatment related effects				
Mating success	No treatment related effects				
Non-pregnant females	2/22	1/22	0/22	0/22	
Corpora lutea			d	d	
Implantation sites				d	
Pre-implantation loss		ic			
Post-implantation loss		ic	ic		
Resorptions	No treatment related effects				
Foetal evaluation (F2)					
Number of litters evaluated	20	20	19	22	
Number of live foetuses	No treatment related effects				
Weight/sex/external abnormalities	No treatment related effects				

(A) Erythema was seen during the treatment period, but turned out to be completely reversible.
(B) Incidental significant increases of water consumption were seen at the highest dose groups.
(C) Slight keratinisation of the skin in females treated with 3.5 and 7.0%.
(D) An increased incidence of hydroureter and hydronephrosis in the 3.5% group was considered to be unrelated to treatment.
(E) The decrease in mean foetal weight was caused by very low weights of the pups in one litter only.

Conclusions NOAEL for maternal toxicity and reproductive effects > 7%.

Rev. note
1. The slightly decreased number of copora lutea and/or implantation sites in the F1 of females treated at 3.5 and/or 7% remained within historical control values.
2. The significant post-implantation loss in the F1 of the lower dosed females was not considered to be related to treatment, but due to total litter loss from one female at 1.75% and 3 females at 3.5%.
3. No information on the use of a (semi)occlusive dressing was available. If no dressing is used, some oral intake of the test substance can not be fully excluded.
4. The purity of the test substance is not indicated. Therefore, the actual amount (a.i.) applied can not be calculated.

Reliability 2 Valid with restrictions

8.4.6.2 Reproductive Toxicity

CAS No. 27323-41-7

(a)

Title	Final report on the safety assessment of sodium dodecylbenzenesulfonate/TEA-dodecylbenzenesulfonate/sodiumdecylbenzenesulfonate	
Date of report	1997.	
GLP	No data	
Reference	**1. Cosmetic, Toiletry and Fragrance Association (CTFA).** 1997. CTFA Final report on Na/TEA DDBS.	
Test substance	Benzenesulfonic acid, dodecyl-, compd. with 2,2',2"-nitrilotris(ethanol) (1:1), 0.2-0.3% a.i. in semipermanent hair dye.	
Guideline	Not indicated.	
Stat. method	Not applicable.	
Test system	**Species**	Rat (CD).
	No. of animals	25 males/dose group in the P-group.
	Dosage	Twice weekly dermal application of 0.5 ml/kg to the shaved skin during 10 weeks.
	Procedure	After 10 weeks of dosing, males were mated with untreated females to produce 75 mated females/group. Females were allowed to deliver and 2 healthy 21-day-old F1-males were selected from each litter to mate after 12 weeks with untreated females to produce 300 mated females. These females were killed on day 4-16 of gestation.
	Observations	Number and sex of pups of the F1-generation (live and dead pups) Uteri and offspring of the females mated to F1-males.
Results	No treatment related effects.	
Conclusions	NOAEL > 0.0015 ml/kg bw (equivalent to 1.5 mg/kg bw); only dose	

tested

Reliability 2 Valid with restriction. CTFA Cosmetic Ingredient Review

CAS No. 42615-29-2

(a)

Title	Effect of alcohol sulfate, linear alkylbenzene sulfonate and natural soap on the development of fertilized eggs of the mouse in vitro	
Date of report	1990.	
GLP	No.	
Reference	**7. Ishii Y., Samejima Y., Saji F., Nomura T.** 1990. Effect of alcohol sulfonate and natural soap on the development of fertilized eggs of the mouse in vitro. Mut. Res. 242: 151-155	
Test substance	Benzenesulphonic acid, linear alkyl, purity not indicated.	
Guideline	Not applicable.	
Stat. method	Not indicated.	
Test system	**Cells**	Fertilised mouse embryo cells.
	Test concentration	0.015, 0.025, 0.03 and 0.05% during 1 h. 0.01, 0.025 and 0.05% for 5 days.
	Procedure	*In vitro f*ertilised eggs at the pronucleus stage were incubated in culture medium containing the test substance for 1 h and observed for 5 days, or incubated for all 5 days of development.
	Observations	Embryo development and blastocyst formation frequency
Results	1 hr test: no impairment of development at 0.015% or 0.025%; at ≥0.03% there was no development (1-cell stage). 5 day test: at ≥0.025% there was no development (1-cell stage).	
Conclusion	NOAEL 0.025% (1 hr) and 0.01% (5 day).	
Reliability	2 Valid with restrictions - Secondary literature.	

CAS No. 68584-26-9

(a)

Title	LAS-Mg : Effects upon the reproductive performance of rats treated continuously through two successive generations
Date of report	April 19, 1982.
GLP	No (QA statement included).
Reference	**29. Tesh J.M. & Mc Anulty P.A.** 1980. LAS-Mg: Effects upon the reproductive performance of rats treated continuously through two successive generations. Life Science research, Stock, Essex, UK
Test substance	Magnesium salt of LAS, purity 38% (slurry).
Guideline	Not indicated.
Stat. method	Multiple t-test, Mann-Whitney U-test, chi-square test, Fisher’s test.

Test system	**Species**	Rat (CD), 30-40 days old, weight 66-90 g (males) and 64-85 g (females).
	No. of animals	P0/F1/F2 12M + 24F/dose level.
	Dosage	Continuous dietary administration at 0, 1250, 2500 and 5000 ppm (nominal a.i.) ⇔ 0, 50, 103 and 222 mg a.i./kg bw (mean measured) during the entire study period.
	Procedures	Males and females were mated (1:2) starting on day 91 (maximum 21 days) to produce the $F1_A$. After ~ 55 days females were re-mated with fresh males to produce the $F1_B$. The detection of a vaginal plug and/or presence of spermatozoa in a vaginal smear was used to define day 1 of gestation. Selected $F1_B$ animals were mated after a maturation period of 91 days according to the same scheme used for the P0 to produce the $F2_A$ and $F2_B$ generation. Selected $F2_B$ animals were killed after a maturation period of 91 days.
	Analyses	In week 0, 26 and 52.
	Observation	Parents • Mortality/clinical signs P0/F1/F2. • Body weight males weekly, females weekly and on day 1,3,7,14 and 21 of gestation and on day 1,7, 14 and 21 after parturation (day 25 (after the second litter only)). • Food and water intake weekly. • Gestation duration/Oestrus cycle. • Macroscopy P0/F1/F2. • Macroscopy (related to neoplasms)/organ weights F2 • histopathology on 5/sex of F2 only (+ on animals with macroscopic findings). Offspring • Clinical signs. • Mortality (visceral examination of dead pups). • Litter size daily until day 21 or 25 (second litters). • Body weight (individually on day 1 and total litter weight on day 4, 10, 14 and 21 (day 25 for second litters)). • Startle response and pupil closure on day 21 or 25 • Macroscopy on pups not selected for the production of the next generation.
Results	**Analyses**	Measured concentration 73-103% of nominal.

Dose (ppm a.i. in diet)	**0**	**1250**	**2500**	**5000**	**DR**
Dose (mean measured mg a.i./kg bw[(A)])	**0**	**50**	**103**	**222**	

	M	F	M	F	M	F	M	F	M	F
P0										
Mortality				1/24	1/12					
Clinical signs			No treatment related effects							
Body weight - wk 13								dc		
- wk 28							d			
- weaning								d		
Food consumption			No treatment related effects							
Water consumption						d		d		
Mating success/fertility			No treatment related effects							
Gestation time/oestrus cycle			No treatment related effects							
Litter size			No treatment related effects							
Live pups (until weaning)			No treatment related effects							
Pup body weight (gain)($F1_A$)			No treatment related effects							
								dc		
($F1_B$)										
Pup clinical signs/behaviour			No treatment related effects							
Pup macroscopy			No treatment related effects							
Parent macroscopy			No treatment related effects							
F1 (selected animals**)**										
Mortality		1/24				1/24				
Clinical signs			No treatment related effects							
Body weight - wk 13								dc		
- weaning								d		
Food/water consumption			No treatment related effects							
Mating success/fertility			No treatment related effects							
Gestation time/oestrus cycle			No treatment related effects							
Litter size ($F2_A$)			No treatment related effects							
($F2_B$) day 0-25				d		d				
Live pups (until weaning) ($F2_A$)			No treatment related effects							
				No treatment related effects						
($F2_B$)										
Pup body weight (gain)($F2_A$)						dc (10%)		dc (21%)		X
			No treatment related effects							
($F2_B$)										
Pup clinical signs/behaviour			No treatment related effects							
Pup macroscopy			No treatment related effects							
Parent macroscopy			No treatment related effects							
F2 (selected animals)										

Mortality			1/24	
Clinical signs	No treatment related effects			
Body weight		d	d	
Food consumption		d		
Water consumption	d	d	d	
Macroscopy	No treatment related effects			
Organ weights				
Heart/spleen		dc[a]		
Lungs/kidneys			dc[a]	
Adrenals			ic[r]	
Prostate		ic[r]		
Histopathology	No treatment related effects			

(A) Based on a mean food intake of 45 mg/kg bw (calculation by the reviewer)

Conclusions "Continuous administration of LAS-Mg to male and female rats, at dietary concentrations of 2500 and 5000 ppm, over two generations, was associated with slight retardation of somatic growth, but there were no adverse effects upon reproductive performance or fertility. The responses of animals receiving LAS-Mg at 1250 ppm were essentially similar to the controls."
NOAEL for reproductive effects is 222 mg a.i./kg bw.
NOAEL based on growth of F2 pups up through lactation is 50 mg a.i./kg bw.

Rev. note
1. The reduced litter size and reduced mean number of live pups in the F2B group treated at 1250 ppm could be attributed to the loss of a single litter.
2. The effects on organ weights were related to the reduced body weights seen in the highest dose group. The increased weight of the adrenals in this group could be attributed to a single female (no macroscopic investigation of this animal was performed). The increased relative prostate weight could be attributed to a single male (macroscopic investigation did not confirm this).

Reliability 1 Valid without restrictions

8.5 Other Relevant Information

CAS No. 68411-30-3

(a)

Type: Toxicokinetics

Method: The absorption, distribution, metabolism and elimination of LAS (radioactively labelled with ^{35}S) were studied in male Charles River rats. LAS was administered as an aqueous solution.

Results: The compound was readily absorbed from the gastrointestinal tract (80-90% of the dose). Most of the absorbed ^{35}S was eliminated within 72 hours and 60-65% of the absorbed dose was eliminated in the urine, with sulfophenyl butanoic and sulfophenyl pentatonic

	acid as metabolites. These metabolites were not reabsorbed from the kidney tubules. 35% of the absorbed ^{35}S was excreted in the bile and were reabsorbed completely from the gastrointestinal tract. Although the metabolites in the bile were not identified, it was shown that no unchanged LAS was eliminated via this pathway.
Test substance:	C_{10-13}, LAS (CAS #**68411-30-3**); alkyl chain length predominately C_{11}, C_{12} and C_{13}.
Remarks:	The authors suggested that metabolism proceeded via omega oxidation with subsequent beta-oxidation. Retention of radioactivity was not observed in any organ.
Reference:	Michael, W.R. 1968. Metabolism of linear alkylate sulfonate and alkyl benzene sulfonate in albino rats. Toxicol. Appl. Pharmacol. 12:473-485.
Reliability:	2 Valid with restrictions

8.6 Abbreviations Used in Robust Summaries

a	Absolute to body weight
-	Absent
+	Present
a.i.	Active ingredient
BP	Boiling point
d	Decrease
dc	Decrease (significant)
DR	Dose related
F	Female
Hb	Haemoglobin
i	Increase
ic	Increase (significant)
M	Male
N/A	Not applicable
r	Relative to body weight
$THCO_2$	Theoretical amount of CO_2
TCO_2	Theoretical amount of CO_2
TS	Test substance
VP	Vapour pressure
WS	Water solubility